Full wwPDB X-ray Structure Validation Report (i)

Aug 15, 2023 – 04:42 PM EDT

PDB ID	:	1XCO
Title	:	Crystal Structure of a Phosphotransacetylase from Bacillus subtilis in complex with acetylphosphate
Authors	:	Xu, Q.S.; Jancarik, J.; Lou, Y.; Yokota, H.; Adams, P.; Kim, R.; Kim, S.-H.; Berkeley Structural Genomics Center (BSGC)
Deposited on	:	2004-09-02
Resolution	:	2.85 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

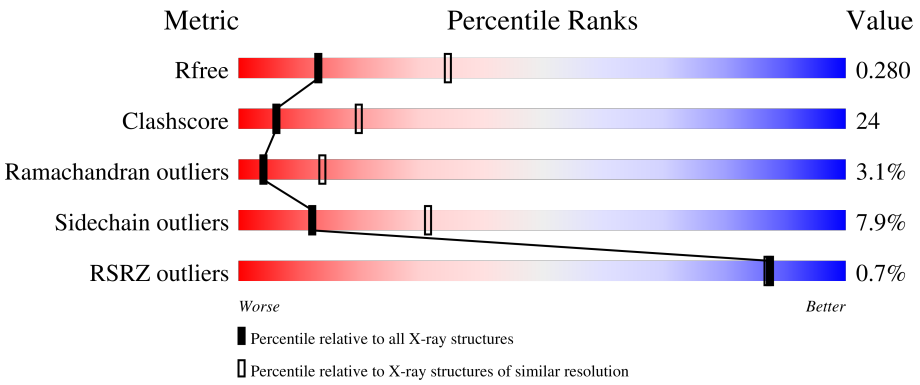
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.85 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3168 (2.90-2.82)
Clashscore	141614	3438 (2.90-2.82)
Ramachandran outliers	138981	3348 (2.90-2.82)
Sidechain outliers	138945	3351 (2.90-2.82)
RSRZ outliers	127900	3103 (2.90-2.82)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	329	58% 34% 6% •
1	B	329	% 57% 36% 5% •
1	C	329	56% 36% 6% •
1	D	329	% 54% 40% 5% •
1	E	329	57% 35% 6% •

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Mol	Chain	Length	Quality of chain
1	F	329	2% 54% 37% 6%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	UVW	D	410	-	-	X	-

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 15000 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Phosphate acetyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	324	2449	1547	408	485	9	0	0	0
1	B	324	2449	1547	408	485	9	0	0	0
1	C	323	2445	1545	407	484	9	0	0	0
1	D	325	2453	1549	409	486	9	0	0	0
1	E	324	2458	1552	409	488	9	0	1	0
1	F	323	2445	1545	407	484	9	0	0	0

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	GLY	-	cloning artifact	UNP P39646
A	-4	GLY	-	cloning artifact	UNP P39646
A	-3	GLY	-	cloning artifact	UNP P39646
A	-2	GLY	-	cloning artifact	UNP P39646
A	-1	GLY	-	cloning artifact	UNP P39646
A	0	GLY	-	cloning artifact	UNP P39646
A	1	MET	-	initiating methionine	UNP P39646
B	-5	GLY	-	cloning artifact	UNP P39646
B	-4	GLY	-	cloning artifact	UNP P39646
B	-3	GLY	-	cloning artifact	UNP P39646
B	-2	GLY	-	cloning artifact	UNP P39646
B	-1	GLY	-	cloning artifact	UNP P39646
B	0	GLY	-	cloning artifact	UNP P39646
B	1	MET	-	initiating methionine	UNP P39646
C	-5	GLY	-	cloning artifact	UNP P39646
C	-4	GLY	-	cloning artifact	UNP P39646
C	-3	GLY	-	cloning artifact	UNP P39646

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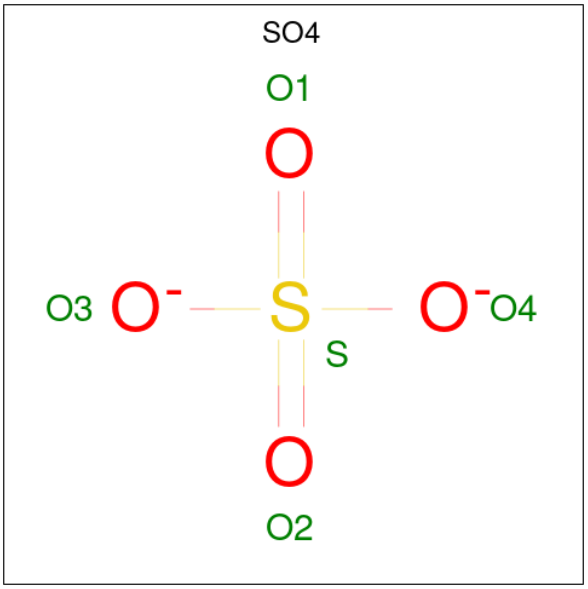
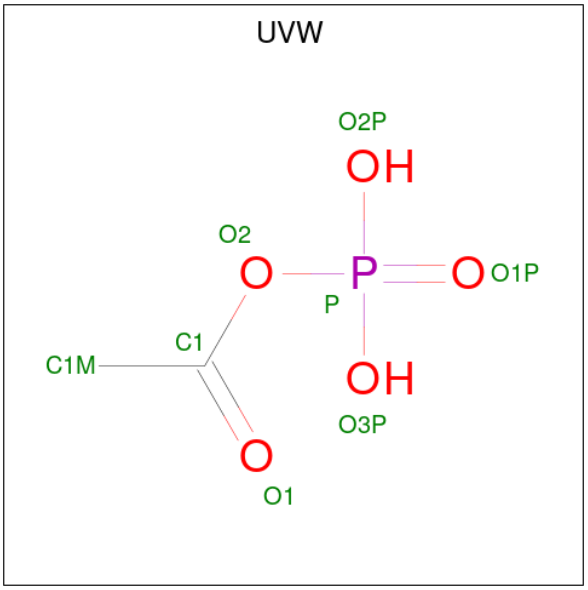
Chain	Residue	Modelled	Actual	Comment	Reference
C	-2	GLY	-	cloning artifact	UNP P39646
C	-1	GLY	-	cloning artifact	UNP P39646
C	0	GLY	-	cloning artifact	UNP P39646
C	1	MET	-	initiating methionine	UNP P39646
D	-5	GLY	-	cloning artifact	UNP P39646
D	-4	GLY	-	cloning artifact	UNP P39646
D	-3	GLY	-	cloning artifact	UNP P39646
D	-2	GLY	-	cloning artifact	UNP P39646
D	-1	GLY	-	cloning artifact	UNP P39646
D	0	GLY	-	cloning artifact	UNP P39646
D	1	MET	-	initiating methionine	UNP P39646
E	-5	GLY	-	cloning artifact	UNP P39646
E	-4	GLY	-	cloning artifact	UNP P39646
E	-3	GLY	-	cloning artifact	UNP P39646
E	-2	GLY	-	cloning artifact	UNP P39646
E	-1	GLY	-	cloning artifact	UNP P39646
E	0	GLY	-	cloning artifact	UNP P39646
E	1	MET	-	initiating methionine	UNP P39646
F	-5	GLY	-	cloning artifact	UNP P39646
F	-4	GLY	-	cloning artifact	UNP P39646
F	-3	GLY	-	cloning artifact	UNP P39646
F	-2	GLY	-	cloning artifact	UNP P39646
F	-1	GLY	-	cloning artifact	UNP P39646
F	0	GLY	-	cloning artifact	UNP P39646
F	1	MET	-	initiating methionine	UNP P39646

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	O	S			
2	A	1	5	4	1		0	0
			Total	O	S			
2	C	1	5	4	1		0	0
			Total	O	S			
2	E	1	5	4	1		0	0

- Molecule 3 is ACETYLPHOSPHATE (three-letter code: UVW) (formula: $C_2H_5O_5P$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	P		
3	A	1	8	2	5	1	0	0
			Total	C	O	P		
3	A	1	8	2	5	1	0	0
			Total	C	O	P		
3	A	1	8	2	5	1	0	0
			Total	C	O	P		
3	A	1	8	2	5	1	0	0
			Total	C	O	P		
3	B	1	8	2	5	1	0	0
			Total	C	O	P		
3	B	1	8	2	5	1	0	0
			Total	C	O	P		
3	B	1	8	2	5	1	0	0
			Total	C	O	P		
3	B	1	8	2	5	1	0	0
			Total	C	O	P		
3	C	1	8	2	5	1	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	P		
3	C	1	8	2	5	1	0	0
			Total	C	O	P		
3	C	1	8	2	5	1	0	0
			Total	C	O	P		
3	C	1	8	2	5	1	0	0
			Total	C	O	P		
3	D	1	8	2	5	1	0	0
			Total	C	O	P		
3	D	1	8	2	5	1	0	0
			Total	C	O	P		
3	D	1	8	2	5	1	0	0
			Total	C	O	P		
3	D	1	8	2	5	1	0	0
			Total	C	O	P		
3	E	1	8	2	5	1	0	0
			Total	C	O	P		
3	E	1	8	2	5	1	0	0
			Total	C	O	P		
3	E	1	8	2	5	1	0	0
			Total	C	O	P		
3	E	1	8	2	5	1	0	0
			Total	C	O	P		
3	F	1	8	2	5	1	0	0
			Total	C	O	P		
3	F	1	8	2	5	1	0	0
			Total	C	O	P		
3	F	1	8	2	5	1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	23	23	23	0	0
			Total	O		
4	B	11	11	11	0	0
			Total	O		
4	C	21	21	21	0	0
			Total	O		
4	D	16	16	16	0	0
			Total	O		
4	E	23	23	23	0	0

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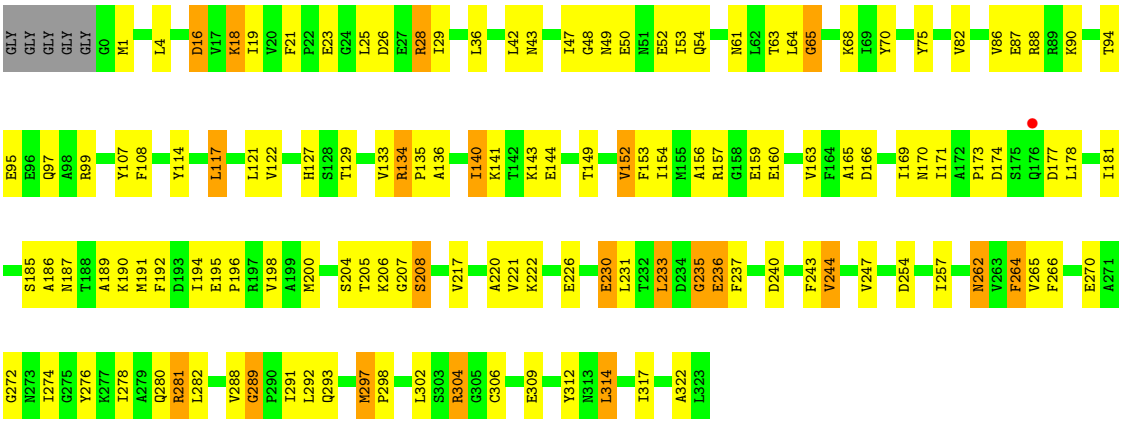
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	F	8	8	8	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

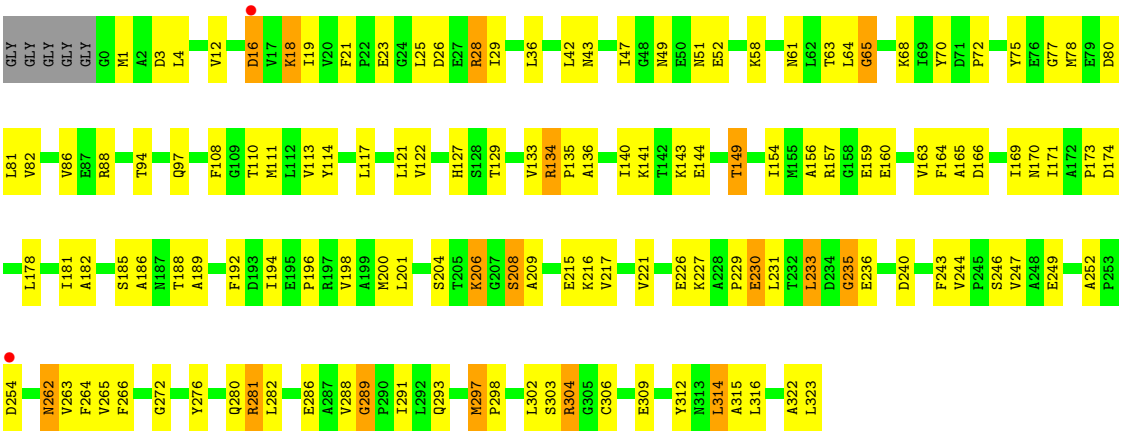
• Molecule 1: Phosphate acetyltransferase

Chain A: 58% 34% 6% •



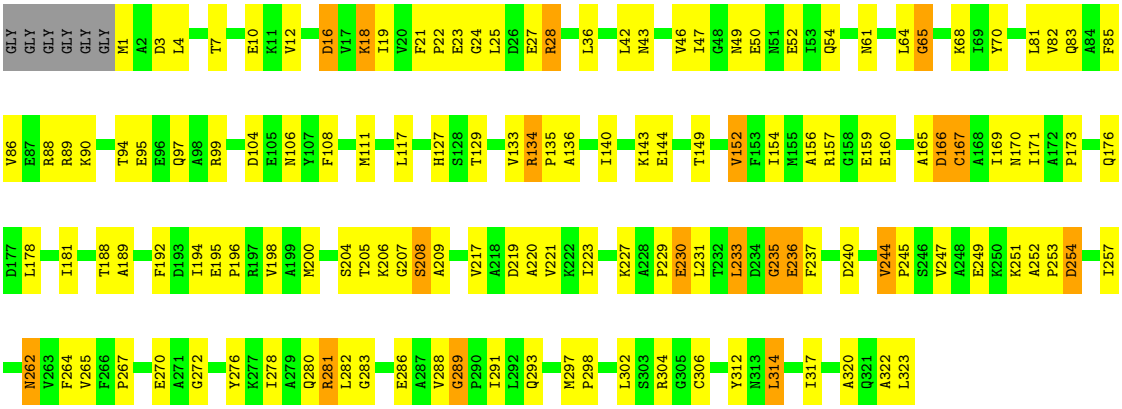
• Molecule 1: Phosphate acetyltransferase

Chain B: % 57% 36% 5% •



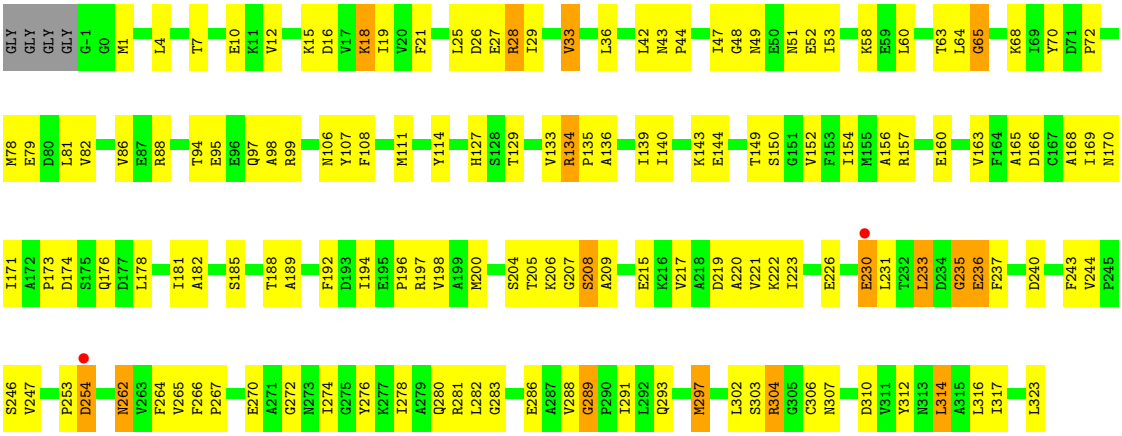
• Molecule 1: Phosphate acetyltransferase

Chain C: 56% 36% 6% •



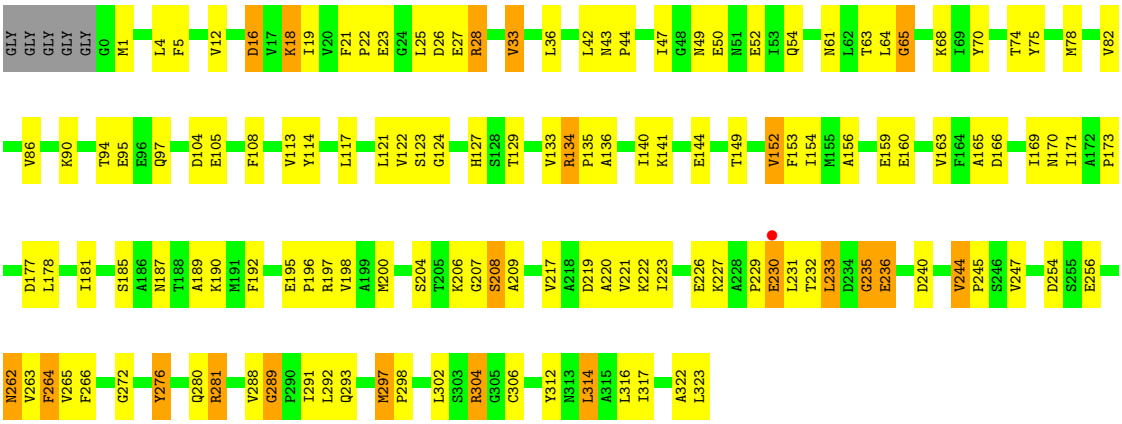
• Molecule 1: Phosphate acetyltransferase

Chain D:



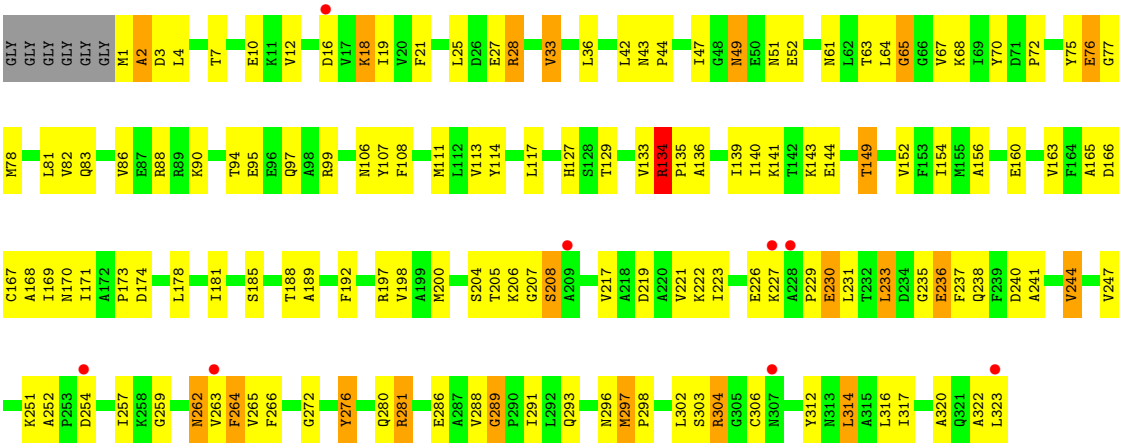
• Molecule 1: Phosphate acetyltransferase

Chain E:



• Molecule 1: Phosphate acetyltransferase

Chain F:


GLY GLY GLY GLY GLY GLY M1 A2 D3 L4 T7 E10 K11 V12 D16 V17 K18 I19 V20 F21 L25 D26 E27 R28 V33 L36 L42 N43 P44 I47 G48 N49 E50 N51 E52 N61 L62 T63 L64 G65 G66 V67 K68 I69 Y70 D71 P72 Y75 E76 G77
M78 L81 V82 Q83 V86 E87 R88 R89 K90 T94 E95 E96 Q97 A98 R99 N106 Y107 F108 M111 L112 V113 Y114 L117 H127 S128 T129 V133 R134 P135 A136 I139 I140 K141 T142 K143 E144 T149 V152 F153 I154 M155 A156 E160 V163 F164 A165 D166
C167 A168 I169 N170 I171 A172 P173 D174 L178 I181 S185 T188 A189 F192 R197 V198 A199 M200 S204 T205 K206 G207 S208 A209 V217 A218 D219 A220 V221 K222 I223 E226 K227 A228 P229 E230 L231 T232 L233 D234 G235 E236 F237 Q238 F239 D240 A241 V244 V247
K251 A252 P253 D254 I257 K258 G259 N262 V263 F264 V265 F266 G272 Y276 Q280 R281 E286 A287 V288 G289 P290 I291 L292 Q293 N296 M297 P298 L302 S303 R304 G305 C306 M307 Y312 N313 L314 A315 L316 I317 A320 Q321 A322 L323

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 64 2 2	Depositor
Cell constants a, b, c, α, β, γ	184.66Å 184.66Å 259.46Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.99 – 2.85 19.99 – 2.85	Depositor EDS
% Data completeness (in resolution range)	99.7 (19.99-2.85) 99.8 (19.99-2.85)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	0.15	Depositor
$< I/\sigma(I) >$ [1]	2.43 (at 2.83Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.245 , 0.288 0.237 , 0.280	Depositor DCC
R_{free} test set	1666 reflections (2.72%)	wwPDB-VP
Wilson B-factor (Å^2)	47.6	Xtriage
Anisotropy	0.486	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 44.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	15000	wwPDB-VP
Average B, all atoms (Å^2)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 54.17 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.7951e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, UVW

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.56	0/2483	0.79	2/3351 (0.1%)
1	B	0.55	0/2483	0.80	1/3351 (0.0%)
1	C	0.57	0/2479	0.78	1/3346 (0.0%)
1	D	0.53	0/2487	0.77	1/3356 (0.0%)
1	E	0.58	0/2492	0.79	1/3363 (0.0%)
1	F	0.50	0/2479	0.75	1/3346 (0.0%)
All	All	0.55	0/14903	0.78	7/20113 (0.0%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	235	GLY	N-CA-C	5.77	127.52	113.10
1	A	235	GLY	N-CA-C	5.64	127.20	113.10
1	C	235	GLY	N-CA-C	5.45	126.71	113.10
1	B	235	GLY	N-CA-C	5.31	126.37	113.10
1	F	238	GLN	N-CA-C	-5.19	96.99	111.00
1	A	140	ILE	N-CA-C	-5.00	97.49	111.00
1	D	235	GLY	N-CA-C	5.00	125.61	113.10

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2449	0	2471	121	0
1	B	2449	0	2471	126	0
1	C	2445	0	2468	123	0
1	D	2453	0	2474	127	0
1	E	2458	0	2476	114	0
1	F	2445	0	2468	129	0
2	A	5	0	0	0	0
2	C	5	0	0	0	0
2	E	5	0	0	0	0
3	A	32	0	12	3	0
3	B	32	0	12	6	0
3	C	32	0	12	3	0
3	D	32	0	12	6	0
3	E	32	0	12	8	0
3	F	24	0	9	1	0
4	A	23	0	0	1	0
4	B	11	0	0	2	0
4	C	21	0	0	2	0
4	D	16	0	0	1	0
4	E	23	0	0	2	0
4	F	8	0	0	0	0
All	All	15000	0	14897	728	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 24.

All (728) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:403:UVW:C1	3:B:403:UVW:O2	1.65	1.44
3:C:420:UVW:O2	3:C:420:UVW:C1	1.64	1.44
3:D:421:UVW:C1	3:D:421:UVW:O2	1.64	1.43
3:D:410:UVW:C1	3:D:410:UVW:O2	1.64	1.42
3:E:413:UVW:C1	3:E:413:UVW:O2	1.63	1.42
3:E:415:UVW:C1	3:E:415:UVW:O2	1.63	1.40
3:E:422:UVW:C1	3:E:422:UVW:O2	1.65	1.40
1:C:165:ALA:HB3	1:C:265:VAL:HA	1.33	1.08
1:C:204:SER:HB2	1:C:208:SER:HB2	1.37	1.07
1:F:198:VAL:HB	1:F:233:LEU:HB2	1.36	1.06
1:A:165:ALA:HB3	1:A:265:VAL:HA	1.32	1.06
1:D:165:ALA:HB3	1:D:265:VAL:HA	1.36	1.06
1:F:165:ALA:HB3	1:F:265:VAL:HA	1.37	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:204:SER:HB2	1:A:208:SER:HB2	1.35	1.06
1:B:204:SER:HB2	1:B:208:SER:HB2	1.35	1.05
1:B:165:ALA:HB3	1:B:265:VAL:HA	1.40	1.03
3:E:413:UVW:C1	3:E:413:UVW:P	2.46	1.02
1:E:221:VAL:HG21	1:E:235:GLY:HA3	1.37	1.02
1:B:221:VAL:HG21	1:B:235:GLY:HA3	1.37	1.02
3:D:410:UVW:C1	3:D:410:UVW:P	2.47	1.02
1:C:198:VAL:HB	1:C:233:LEU:HB2	1.42	1.01
1:D:204:SER:HB2	1:D:208:SER:HB2	1.40	1.00
1:C:231:LEU:HD12	1:C:233:LEU:HD23	1.42	1.00
1:E:198:VAL:HB	1:E:233:LEU:HB2	1.43	1.00
3:D:421:UVW:C1	3:D:421:UVW:P	2.50	0.99
1:A:198:VAL:HB	1:A:233:LEU:HB2	1.43	0.99
1:E:204:SER:HB2	1:E:208:SER:HB2	1.42	0.98
1:E:165:ALA:HB3	1:E:265:VAL:HA	1.45	0.98
1:C:302:LEU:HD23	1:C:314:LEU:HD12	1.46	0.98
1:D:16:ASP:HB2	1:D:43:ASN:HD21	1.27	0.98
3:E:415:UVW:C1	3:E:415:UVW:P	2.51	0.97
3:E:422:UVW:C1	3:E:422:UVW:P	2.54	0.96
3:B:403:UVW:C1	3:B:403:UVW:P	2.54	0.96
1:F:204:SER:HB2	1:F:208:SER:HB2	1.46	0.95
1:F:302:LEU:HD23	1:F:314:LEU:HD12	1.46	0.94
3:C:420:UVW:C1	3:C:420:UVW:P	2.54	0.94
1:D:198:VAL:HB	1:D:233:LEU:HB2	1.49	0.94
1:A:19:ILE:HG22	1:A:21:PHE:CE1	2.03	0.93
1:B:302:LEU:HD23	1:B:314:LEU:HD12	1.49	0.92
1:B:198:VAL:HB	1:B:233:LEU:HB2	1.52	0.92
1:F:36:LEU:HD13	1:F:42:LEU:HD11	1.53	0.90
1:A:302:LEU:HD23	1:A:314:LEU:HD12	1.53	0.89
1:E:231:LEU:HD12	1:E:233:LEU:HD23	1.54	0.88
1:D:221:VAL:HG21	1:D:235:GLY:HA3	1.53	0.88
1:D:36:LEU:HD13	1:D:42:LEU:HD11	1.56	0.87
1:E:36:LEU:HD13	1:E:42:LEU:HD11	1.56	0.87
1:D:49:ASN:HD22	1:D:52:GLU:H	1.24	0.86
1:D:16:ASP:HB2	1:D:43:ASN:ND2	1.91	0.85
1:F:49:ASN:HD22	1:F:52:GLU:H	1.25	0.85
1:A:141:LYS:HB2	3:A:401:UVW:H1M3	1.57	0.84
1:A:221:VAL:HG21	1:A:235:GLY:HA3	1.58	0.84
1:E:200:MET:HG3	1:E:221:VAL:HG22	1.60	0.84
1:C:129:THR:O	1:C:133:VAL:HG12	1.78	0.83
1:A:134:ARG:HB3	1:A:135:PRO:HD3	1.62	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:16:ASP:HB2	1:B:43:ASN:HD21	1.45	0.81
1:E:221:VAL:CG2	1:E:235:GLY:HA3	2.09	0.81
1:B:221:VAL:CG2	1:B:235:GLY:HA3	2.10	0.80
1:F:231:LEU:HD12	1:F:233:LEU:HD23	1.63	0.80
1:B:19:ILE:HG22	1:B:21:PHE:CE1	2.17	0.80
1:B:231:LEU:HD12	1:B:233:LEU:HD23	1.62	0.80
1:A:231:LEU:HD12	1:A:233:LEU:HD23	1.62	0.80
1:E:19:ILE:HG22	1:E:21:PHE:CE1	2.17	0.79
1:E:16:ASP:HB2	1:E:43:ASN:HD21	1.47	0.79
1:F:302:LEU:CD2	1:F:314:LEU:HD12	2.13	0.79
1:D:231:LEU:HD12	1:D:233:LEU:HD23	1.64	0.78
1:F:16:ASP:HB2	1:F:43:ASN:HD21	1.48	0.78
1:C:49:ASN:HD22	1:C:52:GLU:H	1.31	0.77
1:E:302:LEU:HD23	1:E:314:LEU:HD12	1.67	0.76
1:D:221:VAL:CG2	1:D:235:GLY:HA3	2.15	0.76
1:E:49:ASN:HD22	1:E:52:GLU:H	1.30	0.76
1:F:221:VAL:HG21	1:F:235:GLY:HA3	1.67	0.76
1:A:165:ALA:CB	1:A:265:VAL:HA	2.14	0.76
1:A:36:LEU:HD13	1:A:42:LEU:HD11	1.68	0.76
1:B:49:ASN:HD22	1:B:52:GLU:H	1.34	0.75
1:F:129:THR:O	1:F:133:VAL:HG12	1.86	0.75
1:D:129:THR:O	1:D:133:VAL:HG12	1.87	0.74
1:C:19:ILE:HG22	1:C:21:PHE:CE1	2.22	0.74
1:F:19:ILE:HG22	1:F:21:PHE:CE1	2.22	0.74
1:D:94:THR:HB	1:D:97:GLN:HG3	1.69	0.74
1:D:165:ALA:CB	1:D:265:VAL:HA	2.18	0.73
1:B:16:ASP:HB2	1:B:43:ASN:ND2	2.02	0.73
1:C:221:VAL:HG21	1:C:235:GLY:HA3	1.69	0.73
1:F:49:ASN:ND2	1:F:52:GLU:H	1.86	0.73
1:F:165:ALA:CB	1:F:265:VAL:HA	2.16	0.73
1:B:200:MET:HG3	1:B:221:VAL:HG22	1.70	0.72
1:B:72:PRO:HG3	1:B:108:PHE:CD1	2.25	0.72
1:E:165:ALA:CB	1:E:265:VAL:HA	2.19	0.72
1:F:18:LYS:O	1:F:19:ILE:HD12	1.89	0.72
1:E:129:THR:O	1:E:133:VAL:HG12	1.90	0.71
1:A:49:ASN:HD22	1:A:52:GLU:H	1.39	0.71
1:D:262:ASN:HD22	1:D:262:ASN:H	1.39	0.71
1:B:302:LEU:CD2	1:B:314:LEU:HD12	2.20	0.70
1:D:302:LEU:HD23	1:D:314:LEU:HD12	1.73	0.70
1:A:18:LYS:O	1:A:19:ILE:HD12	1.92	0.69
1:C:36:LEU:HD13	1:C:42:LEU:HD11	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:171:ILE:HD12	1:A:171:ILE:H	1.55	0.69
1:F:169:ILE:HG22	1:F:170:ASN:N	2.07	0.69
1:F:16:ASP:HB2	1:F:43:ASN:ND2	2.08	0.69
1:F:262:ASN:HD22	1:F:262:ASN:H	1.40	0.69
1:D:171:ILE:HD12	1:D:171:ILE:H	1.58	0.69
1:A:68:LYS:HB2	1:A:68:LYS:NZ	2.09	0.68
1:A:221:VAL:CG2	1:A:235:GLY:HA3	2.23	0.67
1:B:36:LEU:HD13	1:B:42:LEU:HD11	1.74	0.67
1:E:262:ASN:H	1:E:262:ASN:HD22	1.43	0.67
1:C:165:ALA:CB	1:C:265:VAL:HA	2.18	0.67
1:F:68:LYS:HB2	1:F:68:LYS:NZ	2.10	0.67
1:D:18:LYS:O	1:D:19:ILE:HD12	1.94	0.67
1:F:221:VAL:CG2	1:F:235:GLY:HA3	2.24	0.67
1:E:61:ASN:HD21	1:F:65:GLY:HA3	1.60	0.67
1:E:16:ASP:HB2	1:E:43:ASN:ND2	2.09	0.66
1:F:81:LEU:HD22	1:F:111:MET:HB3	1.76	0.66
1:F:163:VAL:HG21	1:F:189:ALA:HB2	1.76	0.66
1:E:198:VAL:HB	1:E:233:LEU:CB	2.23	0.66
1:A:61:ASN:HD21	1:D:65:GLY:HA3	1.59	0.66
1:C:221:VAL:CG2	1:C:235:GLY:HA3	2.26	0.66
1:E:47:ILE:HD13	1:E:70:TYR:HB2	1.77	0.66
1:F:165:ALA:HB1	1:F:181:ILE:CG2	2.26	0.66
1:C:157:ARG:NH2	1:D:282:LEU:O	2.28	0.65
1:D:114:TYR:HA	1:D:297:MET:HE2	1.77	0.65
1:E:173:PRO:HB2	1:E:178:LEU:HD22	1.78	0.65
1:F:188:THR:OG1	1:F:293:GLN:NE2	2.29	0.65
1:B:1:MET:O	1:B:4:LEU:HB3	1.96	0.65
1:A:302:LEU:CD2	1:A:314:LEU:HD12	2.26	0.65
1:E:1:MET:CE	1:E:288:VAL:HG23	2.26	0.65
1:A:129:THR:O	1:A:133:VAL:HG12	1.97	0.65
1:B:129:THR:O	1:B:133:VAL:HG12	1.97	0.64
1:C:291:ILE:HD11	1:C:317:ILE:HD13	1.80	0.64
1:F:171:ILE:HD12	1:F:171:ILE:H	1.61	0.64
1:F:198:VAL:HB	1:F:233:LEU:CB	2.21	0.64
1:B:47:ILE:HD13	1:B:70:TYR:HB2	1.79	0.64
1:A:154:ILE:HD13	1:A:291:ILE:HD12	1.78	0.64
1:B:3:ASP:CG	1:D:246:SER:HG	2.01	0.64
1:F:72:PRO:HG3	1:F:108:PHE:CD1	2.33	0.64
1:C:198:VAL:HB	1:C:233:LEU:CB	2.21	0.64
1:E:217:VAL:O	1:E:221:VAL:HG23	1.99	0.63
1:A:94:THR:HG22	1:A:95:GLU:H	1.64	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:200:MET:HG3	1:A:221:VAL:HG22	1.80	0.63
1:B:171:ILE:HD12	1:B:171:ILE:H	1.62	0.63
1:E:1:MET:O	1:E:4:LEU:HB3	1.99	0.63
1:E:50:GLU:O	1:E:54:GLN:HB2	1.99	0.63
1:F:200:MET:HG3	1:F:221:VAL:HG22	1.81	0.63
1:E:163:VAL:HG21	1:E:189:ALA:HB2	1.80	0.63
1:D:19:ILE:HG22	1:D:21:PHE:CE1	2.33	0.63
1:F:82:VAL:O	1:F:86:VAL:HG13	1.99	0.63
1:A:63:THR:HG22	1:A:65:GLY:H	1.64	0.62
1:C:169:ILE:HG22	1:C:170:ASN:N	2.14	0.62
1:C:23:GLU:OE1	1:C:127:HIS:HD2	1.82	0.62
1:D:47:ILE:HD13	1:D:70:TYR:HB2	1.80	0.62
1:D:198:VAL:HB	1:D:233:LEU:CB	2.26	0.62
1:D:114:TYR:HA	1:D:297:MET:CE	2.30	0.62
1:B:280:GLN:HG2	1:B:281:ARG:HD2	1.82	0.62
1:F:312:TYR:HE2	1:F:316:LEU:HD11	1.64	0.62
1:C:302:LEU:CD2	1:C:314:LEU:HD12	2.23	0.62
1:E:227:LYS:O	1:E:229:PRO:HD3	2.00	0.61
1:A:23:GLU:OE1	1:A:127:HIS:HD2	1.82	0.61
1:F:68:LYS:HB2	1:F:68:LYS:HZ2	1.65	0.61
1:F:205:THR:HA	1:F:236:GLU:O	2.00	0.61
1:A:173:PRO:HB2	1:A:178:LEU:HD22	1.81	0.61
1:B:163:VAL:HG21	1:B:189:ALA:HB2	1.82	0.61
1:E:204:SER:HB2	1:E:208:SER:CB	2.26	0.61
1:E:240:ASP:HB3	1:E:247:VAL:HG11	1.81	0.61
1:C:82:VAL:O	1:C:86:VAL:HG13	2.00	0.61
1:D:185:SER:HA	1:D:293:GLN:HE22	1.65	0.61
1:A:198:VAL:HB	1:A:233:LEU:CB	2.26	0.61
1:B:1:MET:CE	1:B:288:VAL:HG23	2.31	0.60
1:C:217:VAL:O	1:C:220:ALA:HB3	2.01	0.60
1:E:230:GLU:CD	1:E:230:GLU:H	1.98	0.60
1:A:26:ASP:HB3	1:A:29:ILE:HD13	1.83	0.60
1:B:169:ILE:HG22	1:B:170:ASN:N	2.17	0.60
1:F:173:PRO:HB2	1:F:178:LEU:HD22	1.84	0.60
1:B:26:ASP:HB3	1:B:29:ILE:HD13	1.83	0.60
1:E:1:MET:O	1:E:4:LEU:N	2.28	0.60
1:C:1:MET:O	1:C:4:LEU:HB3	2.02	0.60
1:D:302:LEU:CD2	1:D:314:LEU:HD12	2.30	0.60
1:B:114:TYR:HA	1:B:297:MET:HE2	1.84	0.59
1:D:68:LYS:HB2	1:D:68:LYS:NZ	2.17	0.59
1:E:28:ARG:HG2	1:E:28:ARG:HH11	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:171:ILE:HD12	1:F:171:ILE:N	2.17	0.59
1:E:94:THR:HG22	1:E:95:GLU:H	1.67	0.59
1:C:200:MET:HG3	1:C:221:VAL:HG22	1.85	0.59
1:E:298:PRO:HG2	1:E:322:ALA:HB2	1.84	0.59
1:A:16:ASP:HB2	1:A:43:ASN:HD21	1.68	0.59
1:A:171:ILE:HD12	1:A:171:ILE:N	2.17	0.59
1:F:28:ARG:HG2	1:F:28:ARG:HH11	1.67	0.59
1:F:1:MET:O	1:F:4:LEU:N	2.29	0.58
1:D:79:GLU:OE2	1:D:99:ARG:NH1	2.37	0.58
1:D:47:ILE:HD12	1:D:108:PHE:CD1	2.39	0.58
1:D:188:THR:OG1	1:D:293:GLN:NE2	2.37	0.58
1:F:217:VAL:O	1:F:221:VAL:HG23	2.04	0.58
1:B:68:LYS:HB2	1:B:68:LYS:NZ	2.19	0.58
1:A:107:TYR:CE1	1:A:135:PRO:HG3	2.39	0.58
1:B:136:ALA:O	1:B:140:ILE:O	2.22	0.58
1:C:88:ARG:NH2	3:C:407:UVW:O3P	2.32	0.58
1:D:169:ILE:HG22	1:D:170:ASN:N	2.18	0.58
1:E:63:THR:HG22	1:E:65:GLY:H	1.67	0.58
1:C:205:THR:HG23	1:C:237:PHE:HA	1.85	0.57
1:F:262:ASN:ND2	1:F:263:VAL:HG23	2.19	0.57
1:F:266:PHE:CD2	1:F:272:GLY:HA2	2.39	0.57
1:C:230:GLU:CD	1:C:230:GLU:H	2.07	0.57
1:C:244:VAL:HG22	1:C:247:VAL:HG23	1.86	0.57
1:E:302:LEU:CD2	1:E:314:LEU:HD12	2.34	0.57
1:B:23:GLU:OE1	1:B:127:HIS:HD2	1.86	0.57
1:E:49:ASN:ND2	1:E:52:GLU:H	2.02	0.57
1:C:291:ILE:CD1	1:C:317:ILE:HD13	2.34	0.57
1:F:156:ALA:HA	1:F:160:GLU:O	2.05	0.57
1:F:280:GLN:HG2	1:F:281:ARG:HD2	1.86	0.57
1:A:281:ARG:HB3	1:B:243:PHE:HD2	1.68	0.57
1:D:94:THR:CB	1:D:97:GLN:HG3	2.35	0.57
1:A:152:VAL:HG11	1:A:293:GLN:NE2	2.20	0.57
1:F:4:LEU:HD11	1:F:154:ILE:HG21	1.87	0.57
1:D:205:THR:HG23	1:D:237:PHE:HA	1.87	0.56
1:B:154:ILE:HD13	1:B:291:ILE:HD12	1.86	0.56
1:D:217:VAL:O	1:D:220:ALA:HB3	2.05	0.56
1:A:230:GLU:CD	1:A:230:GLU:H	2.07	0.56
1:A:240:ASP:CB	1:A:247:VAL:HG11	2.35	0.56
1:B:240:ASP:HB3	1:B:247:VAL:HG11	1.87	0.56
1:E:68:LYS:HB2	1:E:68:LYS:NZ	2.20	0.56
1:D:288:VAL:O	1:D:289:GLY:O	2.22	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:288:VAL:O	1:E:289:GLY:O	2.22	0.56
1:F:165:ALA:HB1	1:F:181:ILE:HG22	1.87	0.56
1:F:262:ASN:H	1:F:262:ASN:ND2	2.03	0.56
1:A:1:MET:CE	1:A:288:VAL:HG23	2.36	0.56
1:A:28:ARG:HH12	1:A:306:CYS:H	1.52	0.56
1:A:114:TYR:HA	1:A:297:MET:HE2	1.87	0.56
1:C:298:PRO:HG2	1:C:322:ALA:HB2	1.87	0.56
1:D:163:VAL:HG21	1:D:189:ALA:HB2	1.86	0.56
1:F:76:GLU:OE2	1:F:76:GLU:N	2.39	0.56
1:A:75:TYR:OH	1:A:117:LEU:HD22	2.06	0.56
1:F:7:THR:O	1:F:10:GLU:HB3	2.05	0.56
1:B:185:SER:HA	1:B:293:GLN:HE22	1.70	0.55
1:E:47:ILE:HD12	1:E:108:PHE:CD1	2.41	0.55
1:D:4:LEU:HD21	1:D:192:PHE:CD2	2.41	0.55
1:D:106:ASN:HD21	1:D:127:HIS:CD2	2.23	0.55
1:E:4:LEU:HD21	1:E:192:PHE:CD2	2.41	0.55
1:A:141:LYS:CB	3:A:401:UVW:H1M3	2.33	0.55
1:B:204:SER:HB2	1:B:208:SER:CB	2.24	0.55
1:F:262:ASN:HD22	1:F:262:ASN:N	2.01	0.55
1:E:82:VAL:O	1:E:86:VAL:HG13	2.06	0.55
1:A:94:THR:CB	1:A:97:GLN:HG3	2.36	0.55
1:A:157:ARG:NH2	1:B:282:LEU:O	2.39	0.55
1:C:205:THR:HA	1:C:236:GLU:O	2.07	0.55
1:A:16:ASP:HB2	1:A:43:ASN:ND2	2.21	0.55
1:E:28:ARG:HH12	1:E:306:CYS:H	1.55	0.55
1:A:240:ASP:HB3	1:A:247:VAL:HG11	1.87	0.55
1:C:95:GLU:HG2	1:C:99:ARG:NH2	2.22	0.55
1:A:28:ARG:HG2	1:A:28:ARG:HH11	1.72	0.54
1:B:134:ARG:HB3	1:B:135:PRO:CD	2.36	0.54
1:E:280:GLN:HG2	1:E:281:ARG:HD2	1.90	0.54
1:E:264:PHE:CD1	1:E:264:PHE:N	2.73	0.54
1:F:312:TYR:CE2	1:F:316:LEU:HD11	2.43	0.54
1:A:121:LEU:HD23	1:A:122:VAL:N	2.22	0.54
1:B:12:VAL:HA	1:B:323:LEU:HD11	1.89	0.54
1:A:4:LEU:HD21	1:A:192:PHE:CD2	2.43	0.54
1:A:280:GLN:HG2	1:A:281:ARG:HD2	1.90	0.54
1:C:188:THR:OG1	1:C:293:GLN:NE2	2.39	0.54
1:C:28:ARG:HG2	1:C:28:ARG:HH11	1.71	0.54
1:D:171:ILE:HD12	1:D:171:ILE:N	2.22	0.54
1:E:23:GLU:OE1	1:E:127:HIS:HD2	1.91	0.54
1:B:165:ALA:CB	1:B:265:VAL:HA	2.26	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:68:LYS:HD3	1:C:70:TYR:CZ	2.43	0.54
1:E:262:ASN:H	1:E:262:ASN:ND2	2.05	0.54
1:C:47:ILE:HD12	1:C:108:PHE:CD1	2.43	0.54
1:E:121:LEU:HD23	1:E:122:VAL:N	2.23	0.54
1:A:94:THR:HB	1:A:97:GLN:HG3	1.89	0.54
1:F:185:SER:HA	1:F:293:GLN:HE22	1.72	0.53
1:A:61:ASN:CA	1:D:63:THR:HB	2.39	0.53
1:A:1:MET:O	1:A:4:LEU:HB3	2.08	0.53
1:B:72:PRO:HG3	1:B:108:PHE:CG	2.42	0.53
1:B:113:VAL:O	1:B:297:MET:HE2	2.07	0.53
1:E:154:ILE:HD13	1:E:291:ILE:HD12	1.91	0.53
1:B:171:ILE:HD12	1:B:171:ILE:N	2.23	0.53
1:F:244:VAL:O	1:F:244:VAL:HG22	2.09	0.53
1:A:61:ASN:ND2	1:D:65:GLY:HA3	2.24	0.53
1:F:291:ILE:HD11	1:F:317:ILE:HD13	1.91	0.53
1:F:107:TYR:CE2	1:F:135:PRO:HB3	2.44	0.53
1:A:288:VAL:O	1:A:289:GLY:O	2.26	0.52
1:D:88:ARG:NH2	3:D:410:UVW:O3P	2.40	0.52
1:E:185:SER:HA	1:E:293:GLN:HE22	1.74	0.52
1:B:110:THR:HG23	1:B:140:ILE:HD11	1.89	0.52
1:E:169:ILE:HG22	1:E:170:ASN:N	2.24	0.52
1:A:28:ARG:HH12	1:A:306:CYS:N	2.07	0.52
1:C:262:ASN:H	1:C:262:ASN:HD22	1.56	0.52
1:E:33:VAL:HG22	1:E:44:PRO:HB2	1.91	0.52
1:F:227:LYS:O	1:F:229:PRO:HD3	2.09	0.52
1:C:7:THR:O	1:C:10:GLU:HB3	2.10	0.52
1:F:78:MET:O	1:F:81:LEU:HB2	2.09	0.52
1:A:264:PHE:N	1:A:264:PHE:CD1	2.76	0.52
1:F:168:ALA:C	1:F:169:ILE:HD12	2.30	0.52
1:B:217:VAL:O	1:B:221:VAL:HG23	2.09	0.52
1:D:200:MET:HG3	1:D:221:VAL:HG22	1.91	0.52
1:E:222:LYS:O	1:E:226:GLU:HB2	2.10	0.52
1:A:304:ARG:HD3	1:A:304:ARG:H	1.75	0.52
1:E:123:SER:OG	1:E:124:GLY:N	2.43	0.52
1:E:171:ILE:H	1:E:171:ILE:HD12	1.75	0.52
1:A:50:GLU:O	1:A:54:GLN:HB2	2.09	0.52
1:B:4:LEU:HD21	1:B:192:PHE:CD2	2.45	0.52
1:B:230:GLU:CD	1:B:230:GLU:H	2.08	0.52
1:B:262:ASN:ND2	1:B:263:VAL:HG23	2.24	0.52
1:D:205:THR:HA	1:D:236:GLU:O	2.10	0.52
1:E:141:LYS:HB2	3:E:413:UVW:H1M3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:68:LYS:HD3	1:A:70:TYR:CZ	2.44	0.51
1:A:88:ARG:NH2	3:A:401:UVW:O3P	2.32	0.51
1:A:95:GLU:HG2	1:A:99:ARG:NH2	2.25	0.51
1:F:94:THR:HB	1:F:97:GLN:HG3	1.91	0.51
1:B:3:ASP:CG	1:D:246:SER:OG	2.48	0.51
1:D:266:PHE:CD2	1:D:272:GLY:HA2	2.45	0.51
1:F:106:ASN:HD21	1:F:127:HIS:CD2	2.29	0.51
1:A:298:PRO:HG2	1:A:322:ALA:HB2	1.92	0.51
1:B:174:ASP:OD1	1:B:174:ASP:C	2.49	0.51
1:B:114:TYR:HA	1:B:297:MET:CE	2.40	0.51
1:C:18:LYS:O	1:C:19:ILE:HD12	2.11	0.51
1:A:61:ASN:C	1:D:63:THR:HB	2.30	0.51
1:B:156:ALA:HA	1:B:160:GLU:O	2.11	0.51
1:F:4:LEU:HD21	1:F:192:PHE:CD2	2.46	0.51
1:F:230:GLU:CD	1:F:230:GLU:H	2.09	0.51
1:E:68:LYS:HD3	1:E:70:TYR:CZ	2.45	0.51
1:F:28:ARG:HH12	1:F:306:CYS:H	1.58	0.51
1:A:217:VAL:O	1:A:221:VAL:HG23	2.11	0.51
1:B:182:ALA:HA	1:B:265:VAL:HG21	1.93	0.51
1:B:298:PRO:HG2	1:B:322:ALA:HB2	1.93	0.51
1:C:49:ASN:ND2	1:C:52:GLU:H	2.03	0.51
1:C:83:GLN:O	1:C:86:VAL:HG22	2.11	0.51
1:D:26:ASP:HB3	1:D:29:ILE:HD13	1.91	0.51
1:D:81:LEU:HD22	1:D:111:MET:HB3	1.91	0.51
1:D:165:ALA:HB1	1:D:181:ILE:CG2	2.41	0.51
1:E:12:VAL:HA	1:E:323:LEU:HD11	1.93	0.51
1:F:1:MET:CE	1:F:288:VAL:HG23	2.41	0.51
1:C:28:ARG:HH12	1:C:306:CYS:H	1.57	0.51
1:A:47:ILE:HD13	1:A:70:TYR:HB2	1.92	0.50
1:A:94:THR:OG1	1:A:97:GLN:HG3	2.11	0.50
1:C:280:GLN:HG2	1:C:281:ARG:HD2	1.92	0.50
1:E:304:ARG:H	1:E:304:ARG:HD3	1.76	0.50
1:C:171:ILE:HD12	1:C:171:ILE:H	1.74	0.50
1:C:264:PHE:CD1	1:C:264:PHE:N	2.78	0.50
1:F:1:MET:HB3	1:F:286:GLU:OE1	2.10	0.50
1:F:222:LYS:O	1:F:226:GLU:HB2	2.10	0.50
1:A:68:LYS:HB2	1:A:68:LYS:HZ3	1.77	0.50
1:B:63:THR:HB	1:C:61:ASN:CA	2.42	0.50
1:B:134:ARG:CB	1:B:135:PRO:CD	2.90	0.50
1:B:240:ASP:CB	1:B:247:VAL:HG11	2.42	0.50
1:D:1:MET:SD	1:D:4:LEU:HD22	2.50	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:18:LYS:O	1:E:19:ILE:HD12	2.12	0.50
1:E:74:THR:O	1:E:75:TYR:C	2.48	0.50
1:F:94:THR:CB	1:F:97:GLN:HG3	2.41	0.50
1:A:134:ARG:CB	1:A:135:PRO:HD3	2.36	0.50
1:B:288:VAL:O	1:B:289:GLY:O	2.29	0.50
1:C:4:LEU:HD21	1:C:192:PHE:CD2	2.47	0.50
1:C:24:GLY:HA2	1:C:46:VAL:HG13	1.94	0.50
1:D:262:ASN:H	1:D:262:ASN:ND2	2.07	0.50
1:F:136:ALA:O	1:F:140:ILE:O	2.29	0.50
1:A:281:ARG:HB3	1:B:243:PHE:CD2	2.46	0.50
1:D:18:LYS:C	1:D:19:ILE:HD12	2.32	0.50
1:D:291:ILE:CD1	1:D:317:ILE:HD13	2.41	0.50
1:F:241:ALA:O	1:F:259:GLY:HA2	2.12	0.50
1:F:264:PHE:CD1	1:F:264:PHE:N	2.78	0.50
1:A:19:ILE:CG2	1:A:21:PHE:CE1	2.88	0.50
1:B:141:LYS:HB2	3:B:404:UVW:H1M3	1.92	0.50
1:E:156:ALA:HA	1:E:160:GLU:O	2.11	0.50
1:B:165:ALA:HB1	1:B:181:ILE:CG2	2.42	0.50
1:B:173:PRO:HB2	1:B:178:LEU:HD22	1.93	0.50
1:B:235:GLY:O	1:B:236:GLU:HB3	2.12	0.50
1:B:312:TYR:HE2	1:B:316:LEU:HD11	1.77	0.50
1:C:47:ILE:HD12	1:C:108:PHE:HD1	1.76	0.50
1:F:94:THR:HG22	1:F:95:GLU:H	1.77	0.50
1:C:176:GLN:HG2	4:C:652:HOH:O	2.11	0.49
1:B:65:GLY:HA3	1:C:61:ASN:HD21	1.76	0.49
1:E:134:ARG:HB3	1:E:135:PRO:CD	2.42	0.49
1:E:262:ASN:ND2	1:E:262:ASN:N	2.60	0.49
1:F:12:VAL:HA	1:F:323:LEU:HD11	1.94	0.49
1:F:18:LYS:C	1:F:19:ILE:HD12	2.32	0.49
1:F:298:PRO:HG2	1:F:322:ALA:HB2	1.93	0.49
1:A:47:ILE:HD12	1:A:108:PHE:CD1	2.46	0.49
1:A:68:LYS:HD3	1:A:70:TYR:CE2	2.47	0.49
1:C:227:LYS:O	1:C:229:PRO:HD3	2.12	0.49
1:F:4:LEU:HD21	1:F:192:PHE:CE2	2.48	0.49
1:F:33:VAL:HG22	1:F:44:PRO:HB2	1.92	0.49
1:C:104:ASP:OD1	1:C:106:ASN:N	2.45	0.49
1:E:136:ALA:O	1:E:140:ILE:O	2.30	0.49
1:F:134:ARG:HG2	1:F:134:ARG:HH11	1.77	0.49
1:D:152:VAL:HG11	1:D:293:GLN:NE2	2.28	0.49
1:D:194:ILE:O	1:D:196:PRO:HD3	2.13	0.49
1:E:219:ASP:O	1:E:223:ILE:HG13	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:47:ILE:HD12	1:D:108:PHE:HD1	1.76	0.49
1:D:72:PRO:HG3	1:D:108:PHE:CD1	2.48	0.49
1:F:231:LEU:CD1	1:F:233:LEU:HB3	2.43	0.49
1:C:154:ILE:N	1:C:154:ILE:HD12	2.28	0.49
1:D:15:LYS:O	1:D:16:ASP:OD2	2.30	0.49
1:D:134:ARG:HG2	1:D:134:ARG:HH11	1.77	0.49
1:D:230:GLU:H	1:D:230:GLU:CD	2.10	0.49
1:F:76:GLU:OE2	1:F:77:GLY:N	2.46	0.49
1:A:187:ASN:O	1:A:190:LYS:HB2	2.13	0.49
1:B:63:THR:HG22	1:B:65:GLY:H	1.77	0.49
1:D:154:ILE:HD13	1:D:291:ILE:HD12	1.95	0.49
1:D:219:ASP:O	1:D:223:ILE:HG13	2.13	0.49
1:F:244:VAL:HG22	1:F:247:VAL:H	1.78	0.49
1:B:28:ARG:HH12	1:B:306:CYS:H	1.61	0.49
1:C:94:THR:CB	1:C:97:GLN:HG3	2.42	0.49
1:C:136:ALA:O	1:C:140:ILE:O	2.31	0.49
1:D:48:GLY:HA3	1:D:53:ILE:HD11	1.93	0.49
1:F:317:ILE:O	1:F:320:ALA:HB3	2.13	0.48
1:A:136:ALA:O	1:A:140:ILE:O	2.32	0.48
1:C:94:THR:OG1	1:C:97:GLN:HG3	2.13	0.48
1:C:207:GLY:O	1:C:208:SER:C	2.51	0.48
1:C:270:GLU:OE2	1:D:267:PRO:HB2	2.13	0.48
1:E:68:LYS:HD3	1:E:70:TYR:CE2	2.48	0.48
1:B:134:ARG:HH11	1:B:134:ARG:HG2	1.78	0.48
1:F:262:ASN:ND2	1:F:262:ASN:N	2.61	0.48
1:D:7:THR:O	1:D:10:GLU:HB3	2.13	0.48
1:E:114:TYR:HA	1:E:297:MET:CE	2.43	0.48
1:E:262:ASN:HD22	1:E:262:ASN:N	2.04	0.48
1:D:1:MET:CE	1:D:288:VAL:HG23	2.44	0.48
1:D:4:LEU:HD11	1:D:154:ILE:HG21	1.96	0.48
1:F:197:ARG:N	1:F:262:ASN:HD21	2.11	0.48
1:A:152:VAL:HG23	1:A:153:PHE:N	2.28	0.48
1:B:262:ASN:C	1:B:262:ASN:HD22	2.17	0.48
1:A:233:LEU:C	1:A:233:LEU:HD12	2.34	0.48
1:B:303:SER:O	1:B:304:ARG:C	2.52	0.48
1:A:156:ALA:HA	1:A:160:GLU:O	2.13	0.48
1:B:82:VAL:O	1:B:86:VAL:HG13	2.14	0.48
1:B:141:LYS:CB	3:B:404:UVW:H1M3	2.43	0.48
1:E:114:TYR:HA	1:E:297:MET:HE2	1.95	0.48
1:A:114:TYR:HA	1:A:297:MET:CE	2.44	0.48
1:D:168:ALA:C	1:D:169:ILE:HD12	2.35	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:28:ARG:HH11	1:D:28:ARG:HG2	1.78	0.47
1:E:63:THR:HG22	1:E:65:GLY:N	2.29	0.47
1:E:105:GLU:HG2	4:E:639:HOH:O	2.12	0.47
1:E:197:ARG:N	1:E:262:ASN:HD21	2.11	0.47
1:E:235:GLY:O	1:E:236:GLU:HB3	2.13	0.47
1:F:47:ILE:HD13	1:F:70:TYR:HB2	1.95	0.47
1:C:81:LEU:HD22	1:C:111:MET:HB3	1.95	0.47
1:E:227:LYS:C	1:E:229:PRO:HD3	2.34	0.47
1:B:264:PHE:CD1	1:B:264:PHE:N	2.82	0.47
1:B:309:GLU:O	1:B:309:GLU:HG2	2.14	0.47
1:D:274:ILE:O	1:D:278:ILE:HG13	2.14	0.47
1:A:314:LEU:HD23	1:A:314:LEU:HA	1.69	0.47
1:C:281:ARG:HB3	1:D:243:PHE:CD2	2.49	0.47
1:B:81:LEU:HD22	1:B:111:MET:HB3	1.97	0.47
1:B:233:LEU:HD12	1:B:233:LEU:C	2.35	0.47
1:C:1:MET:CE	1:C:288:VAL:HG23	2.45	0.47
1:C:68:LYS:HB2	1:C:68:LYS:NZ	2.30	0.47
1:C:231:LEU:CD1	1:C:233:LEU:HB3	2.45	0.47
1:C:235:GLY:O	1:C:236:GLU:HB3	2.15	0.47
1:D:182:ALA:HA	1:D:265:VAL:HG21	1.97	0.47
1:A:262:ASN:HD22	1:A:262:ASN:H	1.61	0.47
1:B:304:ARG:HD3	3:B:419:UVW:O1P	2.14	0.47
1:C:154:ILE:N	1:C:154:ILE:CD1	2.78	0.47
1:D:72:PRO:HG3	1:D:108:PHE:CG	2.49	0.47
1:D:262:ASN:ND2	1:D:262:ASN:N	2.62	0.47
1:E:169:ILE:N	1:E:169:ILE:HD12	2.30	0.47
1:F:134:ARG:HB3	1:F:135:PRO:CD	2.45	0.47
1:F:174:ASP:OD1	1:F:174:ASP:C	2.54	0.47
1:F:276:TYR:CD1	1:F:276:TYR:C	2.88	0.47
1:C:173:PRO:HB2	1:C:178:LEU:HD22	1.97	0.47
1:B:303:SER:C	1:B:304:ARG:O	2.49	0.46
1:E:312:TYR:HE2	1:E:316:LEU:HD11	1.80	0.46
1:F:140:ILE:HG22	1:F:296:ASN:HB2	1.97	0.46
1:C:68:LYS:HD3	1:C:70:TYR:CE2	2.50	0.46
1:D:12:VAL:HA	1:D:323:LEU:HD11	1.96	0.46
1:D:27:GLU:HB3	1:D:60:LEU:HD11	1.97	0.46
1:D:240:ASP:HB3	1:D:247:VAL:HG11	1.97	0.46
1:F:167:CYS:HB3	1:F:272:GLY:O	2.15	0.46
1:A:152:VAL:CG1	1:A:293:GLN:NE2	2.78	0.46
1:B:64:LEU:HD23	1:B:64:LEU:HA	1.72	0.46
1:C:166:ASP:HB3	4:C:673:HOH:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:171:ILE:HD12	1:C:171:ILE:N	2.30	0.46
1:E:64:LEU:HD23	1:E:64:LEU:HA	1.72	0.46
1:F:237:PHE:CE1	1:F:257:ILE:HB	2.51	0.46
1:F:240:ASP:HB3	1:F:247:VAL:HG11	1.97	0.46
1:A:68:LYS:HB2	1:A:68:LYS:HZ2	1.80	0.46
1:B:165:ALA:HB1	1:B:181:ILE:HG22	1.97	0.46
1:B:201:LEU:HD11	1:B:264:PHE:HB3	1.98	0.46
1:D:307:ASN:HB2	1:D:310:ASP:OD2	2.16	0.46
1:B:88:ARG:HA	4:B:607:HOH:O	2.16	0.46
1:B:169:ILE:N	1:B:169:ILE:HD12	2.31	0.46
1:D:33:VAL:HG22	1:D:44:PRO:HB2	1.96	0.46
1:B:227:LYS:O	1:B:229:PRO:HD3	2.15	0.46
1:D:154:ILE:HD12	1:D:154:ILE:N	2.30	0.46
1:D:280:GLN:HG2	1:D:281:ARG:HD2	1.97	0.46
1:F:95:GLU:HG2	1:F:99:ARG:HH22	1.80	0.46
1:A:47:ILE:HD12	1:A:108:PHE:HD1	1.79	0.46
1:C:231:LEU:HD12	1:C:233:LEU:CD2	2.30	0.46
1:D:58:LYS:HD2	4:D:612:HOH:O	2.16	0.46
1:E:187:ASN:O	1:E:190:LYS:HB2	2.16	0.46
1:B:1:MET:HB3	1:B:286:GLU:OE1	2.16	0.46
1:A:243:PHE:CZ	1:B:282:LEU:HD21	2.50	0.46
1:B:314:LEU:HD23	1:B:314:LEU:HA	1.72	0.46
1:C:278:ILE:HG23	1:C:282:LEU:HD12	1.97	0.45
1:A:237:PHE:CE1	1:A:257:ILE:HB	2.50	0.45
1:D:49:ASN:HD21	1:D:51:ASN:HB2	1.81	0.45
1:E:291:ILE:CD1	1:E:317:ILE:HD13	2.46	0.45
1:B:94:THR:HB	1:B:97:GLN:HG3	1.97	0.45
1:D:204:SER:HB2	1:D:209:ALA:H	1.81	0.45
1:F:83:GLN:O	1:F:86:VAL:HG22	2.16	0.45
1:F:149:THR:HG23	1:F:293:GLN:O	2.16	0.45
1:A:205:THR:HA	1:A:236:GLU:O	2.16	0.45
1:C:95:GLU:HG2	1:C:99:ARG:HH22	1.81	0.45
1:C:134:ARG:HG2	1:C:134:ARG:HH11	1.82	0.45
1:E:314:LEU:HA	1:E:314:LEU:HD23	1.61	0.45
1:F:227:LYS:C	1:F:229:PRO:HD3	2.37	0.45
1:B:75:TYR:CE1	1:B:77:GLY:HA3	2.51	0.45
1:E:47:ILE:HD12	1:E:108:PHE:HD1	1.82	0.45
1:E:134:ARG:CB	1:E:135:PRO:CD	2.94	0.45
1:F:114:TYR:HA	1:F:297:MET:HE2	1.97	0.45
1:F:288:VAL:O	1:F:289:GLY:O	2.35	0.45
1:A:169:ILE:HG22	1:A:170:ASN:N	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:270:GLU:O	1:A:274:ILE:HG13	2.16	0.45
1:B:157:ARG:NH1	1:D:157:ARG:NH1	2.64	0.45
1:C:4:LEU:HD23	1:C:4:LEU:C	2.37	0.45
1:C:94:THR:HB	1:C:97:GLN:HG3	1.99	0.45
1:C:94:THR:HG22	1:C:95:GLU:H	1.81	0.45
1:C:28:ARG:HG2	1:C:28:ARG:NH1	2.32	0.45
1:E:94:THR:HB	1:E:97:GLN:HG3	1.99	0.45
3:E:415:UVW:O2	3:E:415:UVW:C1M	2.45	0.45
1:F:235:GLY:O	1:F:236:GLU:HB3	2.17	0.45
1:E:22:PRO:HD2	1:E:123:SER:HB2	1.98	0.45
1:A:237:PHE:HE1	1:A:257:ILE:HB	1.81	0.45
1:A:281:ARG:HG3	1:A:281:ARG:HH11	1.81	0.45
1:A:309:GLU:HB2	4:A:659:HOH:O	2.16	0.45
1:D:107:TYR:CZ	1:D:135:PRO:HB3	2.51	0.45
1:E:266:PHE:CD2	1:E:272:GLY:HA2	2.52	0.45
1:C:288:VAL:O	1:C:289:GLY:O	2.35	0.45
1:D:197:ARG:HB2	1:D:262:ASN:ND2	2.32	0.45
1:D:303:SER:C	1:D:304:ARG:O	2.54	0.45
1:C:283:GLY:HA2	1:D:283:GLY:HA2	1.99	0.44
1:D:78:MET:O	1:D:82:VAL:HG23	2.17	0.44
1:D:314:LEU:HD23	1:D:314:LEU:HA	1.68	0.44
1:E:68:LYS:HB2	1:E:68:LYS:HZ3	1.81	0.44
1:F:141:LYS:H	1:F:296:ASN:HD22	1.64	0.44
1:F:291:ILE:CD1	1:F:317:ILE:HD13	2.46	0.44
1:A:185:SER:HA	1:A:293:GLN:HE22	1.82	0.44
1:B:18:LYS:O	1:B:19:ILE:HD12	2.17	0.44
1:C:50:GLU:O	1:C:54:GLN:HB2	2.17	0.44
1:D:156:ALA:HA	1:D:160:GLU:O	2.17	0.44
1:A:28:ARG:HG2	1:A:28:ARG:NH1	2.32	0.44
1:A:82:VAL:O	1:A:86:VAL:HG13	2.18	0.44
1:A:86:VAL:CG2	1:A:87:GLU:N	2.81	0.44
1:B:88:ARG:NH2	3:B:404:UVW:O3P	2.36	0.44
1:C:23:GLU:OE1	1:C:127:HIS:CD2	2.68	0.44
1:D:28:ARG:HH12	1:D:306:CYS:H	1.64	0.44
1:B:216:LYS:HE2	1:B:216:LYS:HB3	1.82	0.44
1:C:262:ASN:HD22	1:C:262:ASN:N	2.14	0.44
1:E:204:SER:HB2	1:E:209:ALA:H	1.83	0.44
1:F:314:LEU:HD23	1:F:314:LEU:HA	1.79	0.44
1:B:4:LEU:HD21	1:B:192:PHE:CE2	2.52	0.44
1:A:244:VAL:O	1:A:244:VAL:HG22	2.16	0.44
1:C:18:LYS:C	1:C:19:ILE:HD12	2.38	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:83:GLN:NE2	1:C:86:VAL:HG21	2.32	0.44
1:D:207:GLY:O	1:D:208:SER:C	2.56	0.44
1:D:217:VAL:O	1:D:221:VAL:HG23	2.17	0.44
1:F:204:SER:HB2	1:F:208:SER:CB	2.32	0.44
1:A:26:ASP:OD2	1:A:28:ARG:HB2	2.18	0.44
1:D:303:SER:O	1:D:304:ARG:C	2.56	0.44
1:E:207:GLY:O	1:E:208:SER:C	2.57	0.44
1:F:76:GLU:OE2	1:F:76:GLU:CA	2.65	0.44
1:F:244:VAL:HG22	1:F:247:VAL:HG23	1.99	0.44
1:A:262:ASN:HD22	1:A:262:ASN:C	2.22	0.44
1:C:134:ARG:HB3	1:C:135:PRO:CD	2.48	0.44
1:C:227:LYS:C	1:C:229:PRO:HD3	2.37	0.44
1:D:264:PHE:CD1	1:D:264:PHE:N	2.85	0.44
1:B:204:SER:HB2	1:B:209:ALA:H	1.82	0.43
1:C:156:ALA:HA	1:C:160:GLU:O	2.18	0.43
1:C:237:PHE:CE1	1:C:257:ILE:HB	2.53	0.43
1:D:291:ILE:HD13	1:D:317:ILE:HD13	2.00	0.43
1:E:28:ARG:HG2	1:E:28:ARG:NH1	2.31	0.43
1:E:240:ASP:CB	1:E:247:VAL:HG11	2.45	0.43
1:B:68:LYS:HD3	1:B:70:TYR:CZ	2.53	0.43
1:C:152:VAL:HG11	1:C:293:GLN:NE2	2.33	0.43
1:D:288:VAL:O	1:D:288:VAL:HG12	2.17	0.43
1:E:262:ASN:ND2	1:E:263:VAL:HG23	2.33	0.43
1:F:28:ARG:HG2	1:F:28:ARG:NH1	2.31	0.43
1:A:64:LEU:HA	1:A:64:LEU:HD23	1.74	0.43
1:A:222:LYS:O	1:A:226:GLU:HB2	2.18	0.43
1:B:149:THR:HG23	1:B:293:GLN:O	2.18	0.43
1:D:1:MET:HB3	1:D:286:GLU:OE1	2.18	0.43
1:D:1:MET:HE2	1:D:288:VAL:HG23	2.01	0.43
1:B:49:ASN:HD21	1:B:51:ASN:HB2	1.83	0.43
1:B:171:ILE:H	1:B:171:ILE:CD1	2.30	0.43
1:C:249:GLU:O	1:C:253:PRO:HD3	2.17	0.43
1:E:171:ILE:HD12	1:E:171:ILE:N	2.33	0.43
1:F:219:ASP:O	1:F:223:ILE:HG13	2.18	0.43
1:A:163:VAL:HG21	1:A:189:ALA:HB2	2.00	0.43
1:B:3:ASP:OD1	1:D:246:SER:OG	2.34	0.43
1:D:4:LEU:HD21	1:D:192:PHE:CE2	2.52	0.43
1:D:152:VAL:CG1	1:D:293:GLN:NE2	2.82	0.43
1:F:205:THR:HG23	1:F:237:PHE:HA	1.99	0.43
1:C:4:LEU:HD11	1:C:154:ILE:HG21	2.00	0.43
1:C:16:ASP:HB2	1:C:43:ASN:ND2	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:177:ASP:O	1:E:181:ILE:HG13	2.18	0.43
1:F:303:SER:O	1:F:304:ARG:C	2.56	0.43
1:A:36:LEU:HD23	1:A:312:TYR:CE1	2.54	0.43
1:A:61:ASN:O	1:D:63:THR:HB	2.18	0.43
1:A:235:GLY:O	1:A:236:GLU:HB3	2.19	0.43
1:A:278:ILE:O	1:A:282:LEU:HB2	2.19	0.43
1:B:68:LYS:HD3	1:B:70:TYR:CE2	2.54	0.43
1:C:167:CYS:HB3	1:C:272:GLY:O	2.19	0.43
1:C:221:VAL:HG21	1:C:235:GLY:CA	2.46	0.43
3:D:410:UVW:O2	3:D:410:UVW:C1M	2.46	0.43
1:F:134:ARG:CB	1:F:135:PRO:CD	2.96	0.43
1:F:251:LYS:O	1:F:252:ALA:HB2	2.19	0.43
1:A:217:VAL:O	1:A:220:ALA:HB3	2.19	0.43
1:B:47:ILE:HD12	1:B:108:PHE:CD1	2.54	0.43
1:E:232:THR:HG23	1:E:256:GLU:HB3	2.01	0.43
1:C:64:LEU:HD23	1:C:64:LEU:HA	1.83	0.43
1:C:317:ILE:O	1:C:320:ALA:HB3	2.18	0.43
1:D:136:ALA:O	1:D:140:ILE:O	2.37	0.43
1:A:95:GLU:HG2	1:A:99:ARG:HH22	1.83	0.43
1:B:75:TYR:OH	1:B:117:LEU:HD22	2.19	0.43
1:B:206:LYS:HD3	1:B:252:ALA:HB1	2.01	0.43
1:D:94:THR:HG22	1:D:95:GLU:H	1.84	0.43
1:F:207:GLY:O	1:F:208:SER:C	2.57	0.43
1:B:188:THR:OG1	1:B:293:GLN:NE2	2.52	0.42
1:C:1:MET:HB3	1:C:286:GLU:OE1	2.19	0.42
1:E:61:ASN:C	1:F:63:THR:HB	2.39	0.42
1:F:198:VAL:CG2	1:F:231:LEU:HD11	2.49	0.42
1:A:266:PHE:CD2	1:A:272:GLY:HA2	2.55	0.42
1:B:154:ILE:N	1:B:154:ILE:HD12	2.34	0.42
1:B:312:TYR:CE2	1:B:316:LEU:HD11	2.54	0.42
1:D:240:ASP:CB	1:D:247:VAL:HG11	2.50	0.42
1:E:1:MET:HE1	1:E:288:VAL:HG23	1.97	0.42
1:F:197:ARG:H	1:F:262:ASN:HD21	1.66	0.42
1:A:189:ALA:O	1:A:194:ILE:HB	2.20	0.42
1:C:219:ASP:O	1:C:223:ILE:HG13	2.20	0.42
1:C:240:ASP:HB3	1:C:247:VAL:HG11	2.00	0.42
1:D:134:ARG:HB3	1:D:135:PRO:CD	2.49	0.42
1:B:63:THR:HB	1:C:61:ASN:C	2.39	0.42
1:B:288:VAL:O	1:B:288:VAL:HG12	2.18	0.42
1:D:253:PRO:O	1:D:254:ASP:HB2	2.20	0.42
1:B:110:THR:HG23	1:B:140:ILE:CD1	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:133:VAL:HG22	1:B:133:VAL:O	2.19	0.42
1:F:49:ASN:ND2	1:F:49:ASN:C	2.73	0.42
1:F:88:ARG:NH2	3:F:416:UVW:O3P	2.34	0.42
1:A:169:ILE:HD11	1:A:292:LEU:HD21	2.02	0.42
1:B:163:VAL:O	1:B:164:PHE:HD2	2.03	0.42
1:C:189:ALA:O	1:C:194:ILE:HB	2.20	0.42
1:E:63:THR:HB	1:F:61:ASN:HA	2.00	0.42
1:F:95:GLU:HG2	1:F:99:ARG:NH2	2.34	0.42
1:F:304:ARG:HD3	1:F:304:ARG:H	1.84	0.42
1:A:48:GLY:HA3	1:A:53:ILE:HD11	2.02	0.42
1:A:207:GLY:O	1:A:208:SER:C	2.58	0.42
1:C:12:VAL:HA	1:C:323:LEU:HD11	2.01	0.42
1:C:165:ALA:HB1	1:C:181:ILE:CG2	2.49	0.42
1:E:154:ILE:HG12	1:E:192:PHE:CZ	2.55	0.42
1:A:240:ASP:HB2	1:A:247:VAL:HG11	2.01	0.42
1:C:36:LEU:HD23	1:C:312:TYR:CE1	2.54	0.42
1:C:195:GLU:OE2	1:C:196:PRO:HD2	2.19	0.42
1:D:64:LEU:HD23	1:D:64:LEU:HA	1.87	0.42
1:F:49:ASN:HD21	1:F:51:ASN:HB2	1.83	0.42
1:C:253:PRO:O	1:C:254:ASP:HB2	2.19	0.42
1:E:217:VAL:O	1:E:220:ALA:HB3	2.19	0.42
1:E:292:LEU:HG	4:E:627:HOH:O	2.18	0.42
1:B:63:THR:HG22	1:C:61:ASN:OD1	2.20	0.42
1:C:85:PHE:CE2	1:C:89:ARG:HG3	2.55	0.42
1:D:262:ASN:HD22	1:D:262:ASN:N	2.01	0.42
1:B:186:ALA:HB1	1:B:231:LEU:HD21	2.02	0.41
1:B:246:SER:O	1:B:249:GLU:HG2	2.20	0.41
1:C:22:PRO:HA	1:C:47:ILE:HB	2.01	0.41
1:E:152:VAL:HG23	1:E:153:PHE:N	2.34	0.41
1:F:1:MET:O	1:F:2:ALA:C	2.58	0.41
1:A:154:ILE:HD12	1:A:154:ILE:N	2.35	0.41
1:D:174:ASP:OD1	1:D:174:ASP:C	2.59	0.41
1:D:196:PRO:O	1:D:197:ARG:HG3	2.20	0.41
1:E:153:PHE:CE2	1:E:276:TYR:CZ	3.08	0.41
1:E:291:ILE:HD11	1:E:317:ILE:HD13	2.01	0.41
1:A:186:ALA:HB1	1:A:231:LEU:HD21	2.00	0.41
1:B:63:THR:CG2	1:C:61:ASN:OD1	2.69	0.41
1:B:194:ILE:O	1:B:196:PRO:HD3	2.21	0.41
1:C:28:ARG:HH12	1:C:306:CYS:N	2.17	0.41
1:C:288:VAL:O	1:C:288:VAL:HG12	2.20	0.41
1:A:177:ASP:O	1:A:181:ILE:HG13	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:227:LYS:C	1:B:229:PRO:HD3	2.41	0.41
1:C:267:PRO:HB2	1:D:270:GLU:OE2	2.21	0.41
1:D:86:VAL:HG12	1:D:98:ALA:HB2	2.02	0.41
1:E:5:PHE:HZ	1:E:288:VAL:CG2	2.34	0.41
1:F:83:GLN:NE2	1:F:86:VAL:HG21	2.36	0.41
1:A:49:ASN:ND2	1:A:52:GLU:H	2.13	0.41
1:D:165:ALA:HB1	1:D:181:ILE:HG22	2.02	0.41
1:E:33:VAL:HG22	1:E:44:PRO:CB	2.50	0.41
1:F:28:ARG:HH12	1:F:306:CYS:N	2.17	0.41
1:C:104:ASP:OD1	1:C:106:ASN:HB2	2.20	0.41
1:C:194:ILE:O	1:C:196:PRO:HD3	2.20	0.41
1:C:204:SER:HB2	1:C:209:ALA:H	1.86	0.41
1:C:231:LEU:HD13	1:C:233:LEU:HB3	2.02	0.41
1:D:134:ARG:CB	1:D:135:PRO:CD	2.99	0.41
1:F:64:LEU:HA	1:F:64:LEU:HD23	1.81	0.41
1:A:191:MET:HE3	1:A:317:ILE:HG23	2.03	0.41
1:B:266:PHE:CD2	1:B:272:GLY:HA2	2.56	0.41
1:C:244:VAL:HG22	1:C:244:VAL:O	2.19	0.41
1:C:251:LYS:O	1:C:252:ALA:HB2	2.21	0.41
1:D:95:GLU:HG2	1:D:99:ARG:HH22	1.85	0.41
1:F:1:MET:O	1:F:4:LEU:HB3	2.21	0.41
1:A:195:GLU:HA	1:A:196:PRO:HD3	1.91	0.41
1:A:243:PHE:HD2	1:B:281:ARG:HB3	1.86	0.41
1:A:262:ASN:HD22	1:A:262:ASN:N	2.17	0.41
1:B:47:ILE:CD1	1:B:70:TYR:HB2	2.48	0.41
1:B:58:LYS:HD2	4:B:649:HOH:O	2.21	0.41
1:B:61:ASN:HD21	1:C:65:GLY:HA3	1.86	0.41
1:B:121:LEU:HD23	1:B:122:VAL:N	2.36	0.41
1:D:49:ASN:ND2	1:D:52:GLU:H	2.04	0.41
1:E:19:ILE:CG2	1:E:21:PHE:CE1	2.98	0.41
1:E:26:ASP:OD2	1:E:28:ARG:HB2	2.21	0.41
1:E:195:GLU:HA	1:E:196:PRO:HD3	1.92	0.41
1:F:129:THR:O	1:F:129:THR:HG22	2.21	0.41
1:A:174:ASP:OD1	1:A:174:ASP:C	2.58	0.41
1:D:176:GLN:NE2	1:D:223:ILE:HD13	2.36	0.41
1:D:222:LYS:O	1:D:226:GLU:HB2	2.20	0.41
1:D:312:TYR:HE2	1:D:316:LEU:HD11	1.86	0.41
1:E:163:VAL:HG21	1:E:189:ALA:CB	2.48	0.41
1:E:244:VAL:HA	1:E:245:PRO:HD3	1.86	0.41
1:B:75:TYR:OH	1:B:117:LEU:CD2	2.69	0.40
1:B:198:VAL:HB	1:B:233:LEU:CB	2.37	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:262:ASN:ND2	1:B:262:ASN:C	2.75	0.40
1:D:173:PRO:HB2	1:D:178:LEU:HD22	2.03	0.40
1:E:5:PHE:HZ	1:E:288:VAL:HG22	1.87	0.40
1:F:65:GLY:C	1:F:67:VAL:H	2.24	0.40
1:F:149:THR:CG2	1:F:293:GLN:O	2.69	0.40
1:A:134:ARG:CB	1:A:135:PRO:CD	2.99	0.40
1:C:244:VAL:HA	1:C:245:PRO:HD3	1.92	0.40
1:E:113:VAL:O	1:E:297:MET:HE2	2.22	0.40
1:E:159:GLU:OE2	1:E:159:GLU:HA	2.21	0.40
1:F:113:VAL:O	1:F:297:MET:HE2	2.22	0.40
1:F:171:ILE:H	1:F:171:ILE:CD1	2.31	0.40
1:C:244:VAL:CG2	1:C:247:VAL:HG23	2.52	0.40
1:C:291:ILE:HD13	1:C:317:ILE:HG21	2.04	0.40
1:D:95:GLU:HG2	1:D:99:ARG:NH2	2.35	0.40
1:E:312:TYR:CE2	1:E:316:LEU:HD11	2.56	0.40
1:C:240:ASP:CB	1:C:247:VAL:HG11	2.51	0.40
1:F:303:SER:C	1:F:304:ARG:O	2.57	0.40
1:B:312:TYR:O	1:B:315:ALA:HB3	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	322/329 (98%)	292 (91%)	20 (6%)	10 (3%)	4 14
1	B	322/329 (98%)	283 (88%)	31 (10%)	8 (2%)	5 18
1	C	321/329 (98%)	289 (90%)	22 (7%)	10 (3%)	4 14
1	D	323/329 (98%)	288 (89%)	26 (8%)	9 (3%)	5 16
1	E	323/329 (98%)	284 (88%)	30 (9%)	9 (3%)	5 16
1	F	321/329 (98%)	280 (87%)	28 (9%)	13 (4%)	3 9

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1932/1974 (98%)	1716 (89%)	157 (8%)	59 (3%)	4 14

All (59) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	65	GLY
1	A	144	GLU
1	A	289	GLY
1	B	65	GLY
1	B	144	GLU
1	B	208	SER
1	B	289	GLY
1	C	65	GLY
1	C	143	LYS
1	C	144	GLU
1	C	206	LYS
1	C	208	SER
1	C	289	GLY
1	D	65	GLY
1	D	144	GLU
1	D	208	SER
1	D	289	GLY
1	E	90	LYS
1	E	144	GLU
1	E	206	LYS
1	E	208	SER
1	E	289	GLY
1	F	65	GLY
1	F	144	GLU
1	F	206	LYS
1	F	208	SER
1	F	289	GLY
1	A	90	LYS
1	A	143	LYS
1	A	206	LYS
1	A	208	SER
1	B	143	LYS
1	B	206	LYS
1	C	236	GLU
1	D	143	LYS
1	D	206	LYS
1	E	65	GLY

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Mol	Chain	Res	Type
1	E	166	ASP
1	E	236	GLU
1	F	143	LYS
1	F	166	ASP
1	A	166	ASP
1	A	236	GLU
1	C	16	ASP
1	C	166	ASP
1	D	166	ASP
1	F	2	ALA
1	F	90	LYS
1	F	236	GLU
1	B	16	ASP
1	B	166	ASP
1	C	90	LYS
1	E	16	ASP
1	A	16	ASP
1	D	236	GLU
1	F	75	TYR
1	F	139	ILE
1	D	139	ILE
1	F	134	ARG

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	257/257 (100%)	238 (93%)	19 (7%)	13	35
1	B	257/257 (100%)	237 (92%)	20 (8%)	12	32
1	C	257/257 (100%)	236 (92%)	21 (8%)	11	29
1	D	257/257 (100%)	240 (93%)	17 (7%)	16	40
1	E	258/257 (100%)	236 (92%)	22 (8%)	10	28
1	F	257/257 (100%)	234 (91%)	23 (9%)	9	26
All	All	1543/1542 (100%)	1421 (92%)	122 (8%)	12	31

All (122) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	LYS
1	A	25	LEU
1	A	28	ARG
1	A	117	LEU
1	A	134	ARG
1	A	149	THR
1	A	152	VAL
1	A	159	GLU
1	A	230	GLU
1	A	233	LEU
1	A	244	VAL
1	A	254	ASP
1	A	262	ASN
1	A	264	PHE
1	A	276	TYR
1	A	281	ARG
1	A	297	MET
1	A	304	ARG
1	A	314	LEU
1	B	18	LYS
1	B	25	LEU
1	B	28	ARG
1	B	78	MET
1	B	80	ASP
1	B	134	ARG
1	B	149	THR
1	B	159	GLU
1	B	215	GLU
1	B	226	GLU
1	B	230	GLU
1	B	233	LEU
1	B	244	VAL
1	B	254	ASP
1	B	262	ASN
1	B	276	TYR
1	B	281	ARG
1	B	297	MET
1	B	304	ARG
1	B	314	LEU
1	C	3	ASP
1	C	18	LYS
1	C	25	LEU

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Mol	Chain	Res	Type
1	C	27	GLU
1	C	28	ARG
1	C	117	LEU
1	C	134	ARG
1	C	149	THR
1	C	152	VAL
1	C	159	GLU
1	C	167	CYS
1	C	230	GLU
1	C	233	LEU
1	C	244	VAL
1	C	254	ASP
1	C	262	ASN
1	C	276	TYR
1	C	281	ARG
1	C	297	MET
1	C	304	ARG
1	C	314	LEU
1	D	18	LYS
1	D	25	LEU
1	D	28	ARG
1	D	33	VAL
1	D	134	ARG
1	D	149	THR
1	D	150	SER
1	D	215	GLU
1	D	230	GLU
1	D	233	LEU
1	D	244	VAL
1	D	254	ASP
1	D	262	ASN
1	D	276	TYR
1	D	297	MET
1	D	304	ARG
1	D	314	LEU
1	E	18	LYS
1	E	25	LEU
1	E	27	GLU
1	E	28	ARG
1	E	33	VAL
1	E	78	MET
1	E	104	ASP

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Mol	Chain	Res	Type
1	E	117	LEU
1	E	134	ARG
1	E	149	THR
1	E	152	VAL
1	E	230	GLU
1	E	233	LEU
1	E	244	VAL
1	E	254	ASP
1	E	262	ASN
1	E	264	PHE
1	E	276	TYR
1	E	281	ARG
1	E	297	MET
1	E	304	ARG
1	E	314	LEU
1	F	3	ASP
1	F	18	LYS
1	F	25	LEU
1	F	27	GLU
1	F	28	ARG
1	F	33	VAL
1	F	49	ASN
1	F	76	GLU
1	F	117	LEU
1	F	134	ARG
1	F	149	THR
1	F	152	VAL
1	F	230	GLU
1	F	233	LEU
1	F	244	VAL
1	F	254	ASP
1	F	262	ASN
1	F	264	PHE
1	F	276	TYR
1	F	281	ARG
1	F	297	MET
1	F	304	ARG
1	F	314	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (48) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	43	ASN
1	A	49	ASN
1	A	83	GLN
1	A	127	HIS
1	A	161	GLN
1	A	262	ASN
1	A	293	GLN
1	B	43	ASN
1	B	49	ASN
1	B	83	GLN
1	B	106	ASN
1	B	127	HIS
1	B	161	GLN
1	B	262	ASN
1	B	280	GLN
1	B	293	GLN
1	C	43	ASN
1	C	49	ASN
1	C	83	GLN
1	C	127	HIS
1	C	161	GLN
1	C	262	ASN
1	C	293	GLN
1	D	43	ASN
1	D	49	ASN
1	D	83	GLN
1	D	127	HIS
1	D	161	GLN
1	D	176	GLN
1	D	262	ASN
1	D	280	GLN
1	D	293	GLN
1	E	43	ASN
1	E	49	ASN
1	E	83	GLN
1	E	127	HIS
1	E	161	GLN
1	E	262	ASN
1	E	284	ASN
1	E	293	GLN
1	F	43	ASN
1	F	49	ASN
1	F	83	GLN

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Mol	Chain	Res	Type
1	F	127	HIS
1	F	161	GLN
1	F	262	ASN
1	F	293	GLN
1	F	296	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

26 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	UVW	E	414	-	6,7,7	3.38	2 (33%)	7,10,10	1.76	1 (14%)
3	UVW	A	406	-	6,7,7	2.95	3 (50%)	7,10,10	1.85	1 (14%)
3	UVW	C	408	-	6,7,7	3.10	3 (50%)	7,10,10	1.61	1 (14%)
3	UVW	E	415	-	6,7,7	3.20	4 (66%)	7,10,10	1.63	1 (14%)
3	UVW	D	411	-	6,7,7	3.42	3 (50%)	7,10,10	1.71	1 (14%)
3	UVW	B	419	-	6,7,7	3.48	4 (66%)	7,10,10	1.91	1 (14%)
3	UVW	A	402	-	6,7,7	3.26	3 (50%)	7,10,10	1.62	1 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	UVW	D	421	-	6,7,7	3.44	4 (66%)	7,10,10	1.81	1 (14%)
3	UVW	A	418	-	6,7,7	3.63	3 (50%)	7,10,10	1.49	1 (14%)
3	UVW	F	423	-	6,7,7	3.35	3 (50%)	7,10,10	1.82	1 (14%)
3	UVW	B	404	-	6,7,7	3.49	3 (50%)	7,10,10	1.63	1 (14%)
3	UVW	E	422	-	6,7,7	3.45	4 (66%)	7,10,10	1.87	1 (14%)
3	UVW	B	405	-	6,7,7	3.21	2 (33%)	7,10,10	1.79	1 (14%)
3	UVW	C	420	-	6,7,7	3.15	3 (50%)	7,10,10	1.96	1 (14%)
3	UVW	C	407	-	6,7,7	3.38	3 (50%)	7,10,10	1.62	1 (14%)
3	UVW	E	413	-	6,7,7	3.11	4 (66%)	7,10,10	1.47	1 (14%)
2	SO4	E	503	-	4,4,4	2.21	1 (25%)	6,6,6	0.90	0
2	SO4	C	502	-	4,4,4	2.23	1 (25%)	6,6,6	0.76	0
3	UVW	F	417	-	6,7,7	3.36	3 (50%)	7,10,10	1.76	1 (14%)
3	UVW	B	403	-	6,7,7	3.00	3 (50%)	7,10,10	1.71	1 (14%)
3	UVW	F	416	-	6,7,7	3.20	3 (50%)	7,10,10	1.57	1 (14%)
3	UVW	C	412	-	6,7,7	3.31	3 (50%)	7,10,10	1.72	1 (14%)
3	UVW	D	410	-	6,7,7	3.09	3 (50%)	7,10,10	1.59	1 (14%)
3	UVW	A	401	-	6,7,7	3.21	3 (50%)	7,10,10	1.52	1 (14%)
3	UVW	D	409	-	6,7,7	3.24	3 (50%)	7,10,10	1.63	1 (14%)
2	SO4	A	501	-	4,4,4	2.19	1 (25%)	6,6,6	0.89	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	UVW	E	414	-	-	0/3/5/5	-
3	UVW	A	406	-	-	1/3/5/5	-
3	UVW	C	408	-	-	0/3/5/5	-
3	UVW	E	415	-	-	0/3/5/5	-
3	UVW	D	411	-	-	1/3/5/5	-
3	UVW	B	419	-	-	1/3/5/5	-
3	UVW	A	402	-	-	0/3/5/5	-
3	UVW	D	421	-	-	0/3/5/5	-
3	UVW	A	418	-	-	0/3/5/5	-
3	UVW	F	423	-	-	0/3/5/5	-
3	UVW	B	404	-	-	0/3/5/5	-
3	UVW	E	422	-	-	0/3/5/5	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	UVW	B	405	-	-	0/3/5/5	-
3	UVW	C	420	-	-	3/3/5/5	-
3	UVW	C	407	-	-	1/3/5/5	-
3	UVW	E	413	-	-	0/3/5/5	-
3	UVW	F	417	-	-	1/3/5/5	-
3	UVW	B	403	-	-	0/3/5/5	-
3	UVW	F	416	-	-	0/3/5/5	-
3	UVW	C	412	-	-	0/3/5/5	-
3	UVW	D	410	-	-	0/3/5/5	-
3	UVW	A	401	-	-	0/3/5/5	-
3	UVW	D	409	-	-	0/3/5/5	-

All (75) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	404	UVW	C1M-C1	-6.79	1.26	1.49
3	D	411	UVW	C1M-C1	-6.66	1.26	1.49
3	A	401	UVW	C1M-C1	-6.64	1.26	1.49
3	F	417	UVW	C1M-C1	-6.63	1.26	1.49
3	F	423	UVW	C1M-C1	-6.57	1.26	1.49
3	E	414	UVW	C1M-C1	-6.53	1.27	1.49
3	B	405	UVW	C1M-C1	-6.51	1.27	1.49
3	E	415	UVW	C1M-C1	-6.49	1.27	1.49
3	D	410	UVW	C1M-C1	-6.46	1.27	1.49
3	E	413	UVW	C1M-C1	-6.40	1.27	1.49
3	C	408	UVW	C1M-C1	-6.40	1.27	1.49
3	D	421	UVW	C1M-C1	-6.39	1.27	1.49
3	D	409	UVW	C1M-C1	-6.36	1.27	1.49
3	C	407	UVW	C1M-C1	-6.31	1.27	1.49
3	A	402	UVW	C1M-C1	-6.29	1.27	1.49
3	B	403	UVW	C1M-C1	-6.27	1.27	1.49
3	C	412	UVW	C1M-C1	-6.24	1.28	1.49
3	B	419	UVW	C1M-C1	-6.20	1.28	1.49
3	A	418	UVW	C1M-C1	-6.10	1.28	1.49
3	F	416	UVW	C1M-C1	-6.05	1.28	1.49
3	C	420	UVW	C1M-C1	-6.05	1.28	1.49
3	A	406	UVW	C1M-C1	-5.95	1.29	1.49
3	E	422	UVW	C1M-C1	-5.86	1.29	1.49
3	A	418	UVW	P-O2	-5.42	1.51	1.59
3	B	419	UVW	P-O2	-4.38	1.52	1.59
3	E	422	UVW	P-O2	-4.37	1.52	1.59
3	C	407	UVW	P-O2	-4.31	1.52	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	502	SO4	O1-S	4.17	1.68	1.46
2	A	501	SO4	O1-S	4.12	1.68	1.46
2	E	503	SO4	O1-S	4.09	1.68	1.46
3	B	404	UVW	P-O2	-4.01	1.53	1.59
3	E	414	UVW	P-O2	-3.94	1.53	1.59
3	D	421	UVW	P-O2	-3.92	1.53	1.59
3	C	412	UVW	P-O2	-3.88	1.53	1.59
3	D	411	UVW	P-O2	-3.72	1.53	1.59
3	F	416	UVW	P-O2	-3.65	1.53	1.59
3	A	402	UVW	P-O2	-3.48	1.53	1.59
3	F	417	UVW	P-O2	-3.44	1.54	1.59
3	D	409	UVW	P-O2	-3.39	1.54	1.59
3	C	420	UVW	P-O2	-3.28	1.54	1.59
3	F	423	UVW	P-O2	-3.27	1.54	1.59
3	B	405	UVW	P-O2	-2.96	1.54	1.59
3	A	401	UVW	P-O2	-2.96	1.54	1.59
3	E	415	UVW	P-O2	-2.80	1.55	1.59
3	B	403	UVW	O1-C1	2.72	1.30	1.20
3	B	419	UVW	P-O2P	-2.72	1.44	1.54
3	D	421	UVW	P-O2P	-2.67	1.44	1.54
3	E	422	UVW	P-O1P	-2.66	1.42	1.50
3	E	422	UVW	P-O2P	-2.62	1.44	1.54
3	C	408	UVW	P-O3P	2.56	1.64	1.54
3	B	403	UVW	P-O3P	2.54	1.64	1.54
3	D	411	UVW	P-O2P	-2.52	1.45	1.54
3	A	406	UVW	O1-C1	2.48	1.30	1.20
3	F	416	UVW	O1-C1	2.47	1.30	1.20
3	A	406	UVW	P-O3P	2.44	1.64	1.54
3	E	413	UVW	P-O2	-2.38	1.55	1.59
3	F	417	UVW	O1-C1	2.38	1.29	1.20
3	D	410	UVW	O1-C1	2.36	1.29	1.20
3	F	423	UVW	P-O2P	-2.32	1.45	1.54
3	C	408	UVW	O1-C1	2.31	1.29	1.20
3	B	404	UVW	O1-C1	2.24	1.29	1.20
3	A	418	UVW	P-O2P	-2.24	1.46	1.54
3	C	412	UVW	O1-C1	2.24	1.29	1.20
3	A	402	UVW	O1-C1	2.22	1.29	1.20
3	C	420	UVW	P-O2P	-2.20	1.46	1.54
3	D	409	UVW	O1-C1	2.19	1.29	1.20
3	E	413	UVW	O1-C1	2.16	1.28	1.20
3	C	407	UVW	O1-C1	2.16	1.28	1.20
3	A	401	UVW	O1-C1	2.14	1.28	1.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	410	UVW	P-O3P	2.14	1.63	1.54
3	E	415	UVW	O1-C1	2.11	1.28	1.20
3	D	421	UVW	P-O1P	-2.05	1.43	1.50
3	B	419	UVW	P-O1P	-2.02	1.44	1.50
3	E	415	UVW	P-O3P	2.01	1.62	1.54
3	E	413	UVW	P-O3P	2.01	1.62	1.54

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	420	UVW	O3P-P-O2	4.68	119.52	105.25
3	B	419	UVW	O3P-P-O2	4.32	118.41	105.25
3	E	422	UVW	O3P-P-O2	4.26	118.24	105.25
3	D	421	UVW	O3P-P-O2	4.23	118.14	105.25
3	F	417	UVW	O3P-P-O2	4.11	117.79	105.25
3	F	423	UVW	O3P-P-O2	4.09	117.70	105.25
3	B	405	UVW	O3P-P-O2	4.08	117.70	105.25
3	A	406	UVW	O3P-P-O2	4.07	117.66	105.25
3	C	412	UVW	O3P-P-O2	4.02	117.51	105.25
3	B	403	UVW	O3P-P-O2	3.93	117.23	105.25
3	B	404	UVW	O3P-P-O2	3.83	116.93	105.25
3	C	407	UVW	O3P-P-O2	3.78	116.78	105.25
3	E	414	UVW	O3P-P-O2	3.78	116.78	105.25
3	D	409	UVW	O3P-P-O2	3.69	116.51	105.25
3	E	415	UVW	O3P-P-O2	3.66	116.40	105.25
3	D	411	UVW	O3P-P-O2	3.64	116.36	105.25
3	C	408	UVW	O3P-P-O2	3.63	116.33	105.25
3	F	416	UVW	O3P-P-O2	3.53	116.00	105.25
3	A	401	UVW	O3P-P-O2	3.48	115.86	105.25
3	D	410	UVW	O3P-P-O2	3.46	115.80	105.25
3	A	402	UVW	O3P-P-O2	3.44	115.73	105.25
3	A	418	UVW	O3P-P-O2	3.21	115.05	105.25
3	E	413	UVW	O3P-P-O2	3.09	114.68	105.25

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	407	UVW	C1-O2-P-O2P
3	F	417	UVW	C1-O2-P-O1P
3	A	406	UVW	C1-O2-P-O1P
3	B	419	UVW	C1-O2-P-O1P

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Mol	Chain	Res	Type	Atoms
3	C	420	UVW	C1-O2-P-O1P
3	D	411	UVW	C1-O2-P-O1P
3	C	420	UVW	C1-O2-P-O2P
3	C	420	UVW	C1-O2-P-O3P

There are no ring outliers.

12 monomers are involved in 27 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	415	UVW	3	0
3	B	419	UVW	1	0
3	D	421	UVW	2	0
3	B	404	UVW	3	0
3	E	422	UVW	2	0
3	C	420	UVW	2	0
3	C	407	UVW	1	0
3	E	413	UVW	3	0
3	B	403	UVW	2	0
3	F	416	UVW	1	0
3	D	410	UVW	4	0
3	A	401	UVW	3	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	324/329 (98%)	-0.48	1 (0%)	94	94	13, 37, 67, 89	0
1	B	324/329 (98%)	-0.31	2 (0%)	89	89	19, 43, 74, 97	0
1	C	323/329 (98%)	-0.47	0	100	100	9, 37, 71, 95	0
1	D	325/329 (98%)	-0.29	2 (0%)	89	89	15, 43, 78, 105	0
1	E	324/329 (98%)	-0.37	1 (0%)	94	94	12, 39, 72, 93	0
1	F	323/329 (98%)	0.18	8 (2%)	57	54	24, 65, 95, 108	0
All	All	1943/1974 (98%)	-0.29	14 (0%)	87	87	9, 43, 82, 108	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	254	ASP	3.4
1	F	227	LYS	2.9
1	D	254	ASP	2.6
1	F	228	ALA	2.5
1	F	209	ALA	2.5
1	B	16	ASP	2.4
1	D	230	GLU	2.4
1	F	16	ASP	2.4
1	B	254	ASP	2.3
1	A	176	GLN	2.2
1	E	230	GLU	2.2
1	F	263	VAL	2.1
1	F	323	LEU	2.0
1	F	307	ASN	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	UVW	C	420	8/8	0.78	0.27	40,50,62,75	8
3	UVW	F	423	8/8	0.83	0.26	19,36,49,57	8
3	UVW	D	421	8/8	0.87	0.26	8,39,47,54	8
3	UVW	E	413	8/8	0.87	0.30	28,48,58,60	8
3	UVW	B	419	8/8	0.87	0.23	27,45,49,55	8
3	UVW	E	422	8/8	0.89	0.24	34,43,58,58	8
3	UVW	F	417	8/8	0.90	0.19	17,29,43,45	8
3	UVW	E	415	8/8	0.90	0.22	15,33,45,52	8
3	UVW	A	406	8/8	0.91	0.21	25,42,52,57	8
3	UVW	A	418	8/8	0.91	0.21	37,44,55,63	8
3	UVW	B	404	8/8	0.92	0.23	36,41,49,50	8
3	UVW	E	414	8/8	0.92	0.27	21,32,49,50	8
3	UVW	D	409	8/8	0.93	0.17	27,36,46,49	8
3	UVW	F	416	8/8	0.93	0.21	39,44,49,51	8
3	UVW	D	411	8/8	0.93	0.26	28,35,43,44	8
3	UVW	B	405	8/8	0.93	0.26	17,33,49,50	8
2	SO4	C	502	5/5	0.94	0.24	42,45,47,49	5
3	UVW	C	408	8/8	0.94	0.20	33,43,53,55	8
3	UVW	C	412	8/8	0.94	0.19	22,35,41,50	8
2	SO4	E	503	5/5	0.94	0.19	33,34,46,53	5
3	UVW	B	403	8/8	0.94	0.19	38,52,58,68	8
3	UVW	A	401	8/8	0.94	0.23	37,42,47,50	8
3	UVW	A	402	8/8	0.94	0.20	24,37,40,46	8
3	UVW	D	410	8/8	0.95	0.27	31,41,48,48	8
2	SO4	A	501	5/5	0.95	0.21	39,39,48,51	5
3	UVW	C	407	8/8	0.96	0.16	23,35,41,46	8

6.5 Other polymers (i)

There are no such residues in this entry.