Full wwPDB X-ray Structure Validation Report (i)

Sep 5, 2023 – 05:00 PM EDT

PDB ID	:	4EV5
Title	:	Crystal structure of copper amine oxidase-1 from Hansenula polymorpha in complex with benzylamine
Authors	:	Klema, V.J.; Solheid, C.J.; Wilmot, C.M.
Deposited on	:	2012-04-25
Resolution	:	2.25 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:

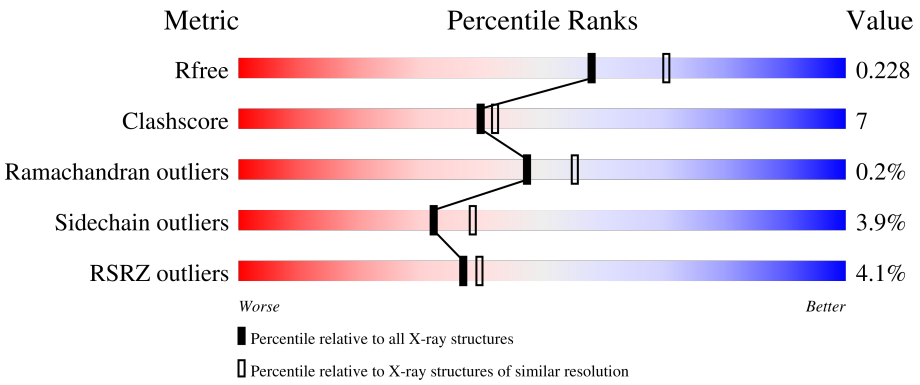
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 2.25 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	1377 (2.26-2.26)
Clashscore	141614	1487 (2.26-2.26)
Ramachandran outliers	138981	1449 (2.26-2.26)
Sidechain outliers	138945	1450 (2.26-2.26)
RSRZ outliers	127900	1356 (2.26-2.26)

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	692	3% 81% 12% • 5%
1	B	692	% 80% 13% • 5%
1	C	692	4% 79% 14% • 5%
1	D	692	9% 79% 14% • 5%
1	E	692	4% 76% 16% • 5%

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Mol	Chain	Length	Quality of chain
1	F	692	3% 81% 12% 5%

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
2	GOL	A	703	-	-	X	-
2	GOL	D	702	-	-	X	-
2	GOL	F	702	-	-	X	-
5	ABN	C	708	-	-	X	-

2 Entry composition (i)

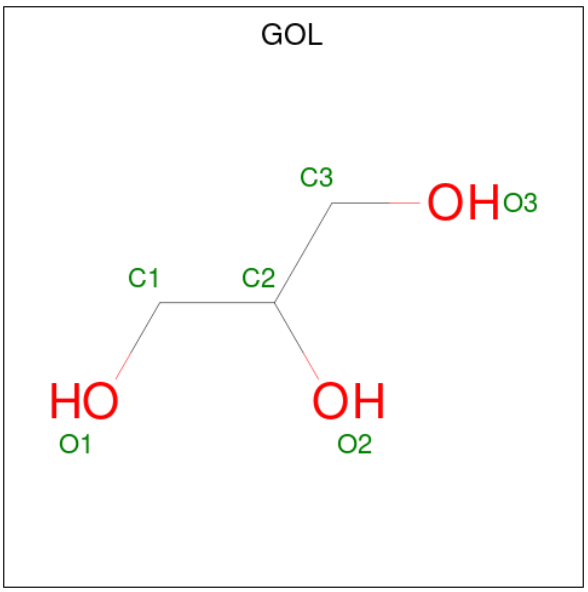
There are 6 unique types of molecules in this entry. The entry contains 34660 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Peroxisomal primary amine oxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	654	5227	3333	891	979	24	0	11	0
1	B	655	5227	3328	897	977	25	0	8	0
1	C	655	5228	3330	891	981	26	0	10	0
1	D	655	5223	3325	896	977	25	0	8	0
1	E	654	5245	3343	899	978	25	0	13	0
1	F	655	5227	3330	896	975	26	0	8	0

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
2	A	1	6	3	3	0	0
2	A	1	6	3	3	0	0
2	A	1	6	3	3	0	0
2	A	1	6	3	3	0	0
2	A	1	6	3	3	0	0
2	B	1	6	3	3	0	0
2	B	1	6	3	3	0	0
2	B	1	6	3	3	0	0
2	B	1	6	3	3	0	0
2	B	1	6	3	3	0	0
2	B	1	6	3	3	0	0
2	C	1	6	3	3	0	0
2	C	1	6	3	3	0	0
2	C	1	6	3	3	0	0
2	C	1	6	3	3	0	0
2	C	1	6	3	3	0	0
2	C	1	6	3	3	0	0
2	D	1	6	3	3	0	0
2	D	1	6	3	3	0	0
2	D	1	6	3	3	0	0
2	D	1	6	3	3	0	0
2	E	1	6	3	3	0	0

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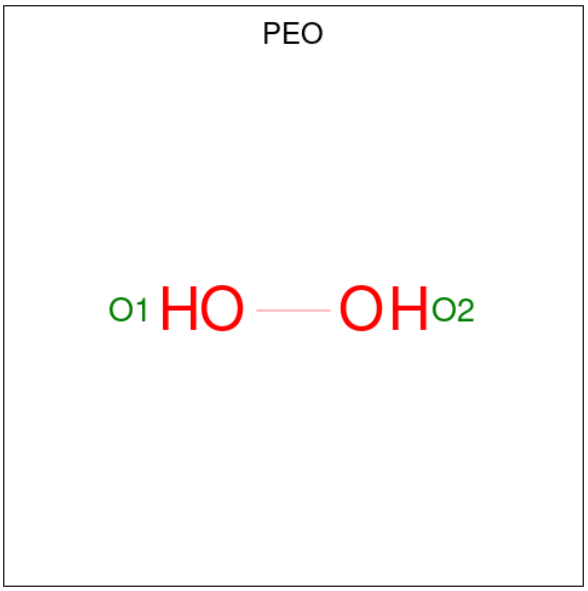
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
2	E	1	6	3	3	0	0
			Total	C	O		
2	E	1	6	3	3	0	0
			Total	C	O		
2	E	1	6	3	3	0	0
			Total	C	O		
2	F	1	6	3	3	0	0
			Total	C	O		
2	F	1	6	3	3	0	0
			Total	C	O		
2	F	1	6	3	3	0	0
			Total	C	O		
2	F	1	6	3	3	0	0
			Total	C	O		
2	F	1	6	3	3	0	0

- Molecule 3 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

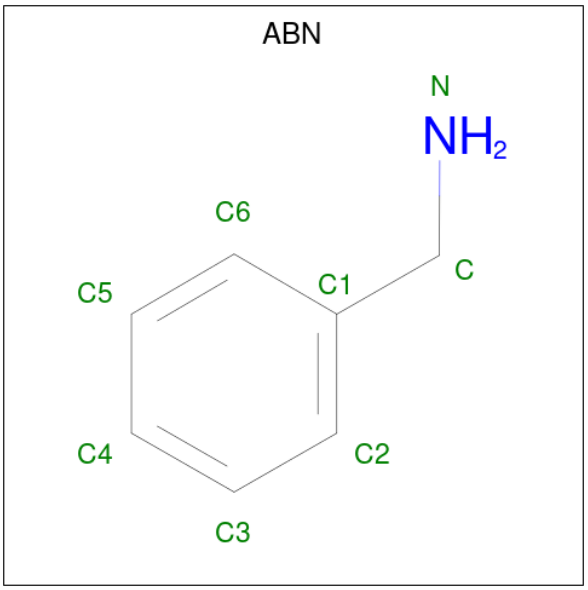
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cu		
3	A	1	1	1	0	0
			Total	Cu		
3	B	1	1	1	0	0
			Total	Cu		
3	C	1	1	1	0	0
			Total	Cu		
3	D	1	1	1	0	0
			Total	Cu		
3	E	1	1	1	0	0
			Total	Cu		
3	F	1	1	1	0	0

- Molecule 4 is HYDROGEN PEROXIDE (three-letter code: PEO) (formula: H_2O_2).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total O 2 2	0	0
4	B	1	Total O 2 2	0	0
4	E	1	Total O 2 2	0	0
4	F	1	Total O 2 2	0	0

- Molecule 5 is BENZYLAMINE (three-letter code: ABN) (formula: C_7H_9N).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	N		
5	A	1	8	7	1	0	0
5	B	1	8	7	1	0	0
5	C	1	8	7	1	0	0
5	D	1	8	7	1	0	0
5	E	1	8	7	1	0	0
5	F	1	8	7	1	0	0

- Molecule 6 is water.

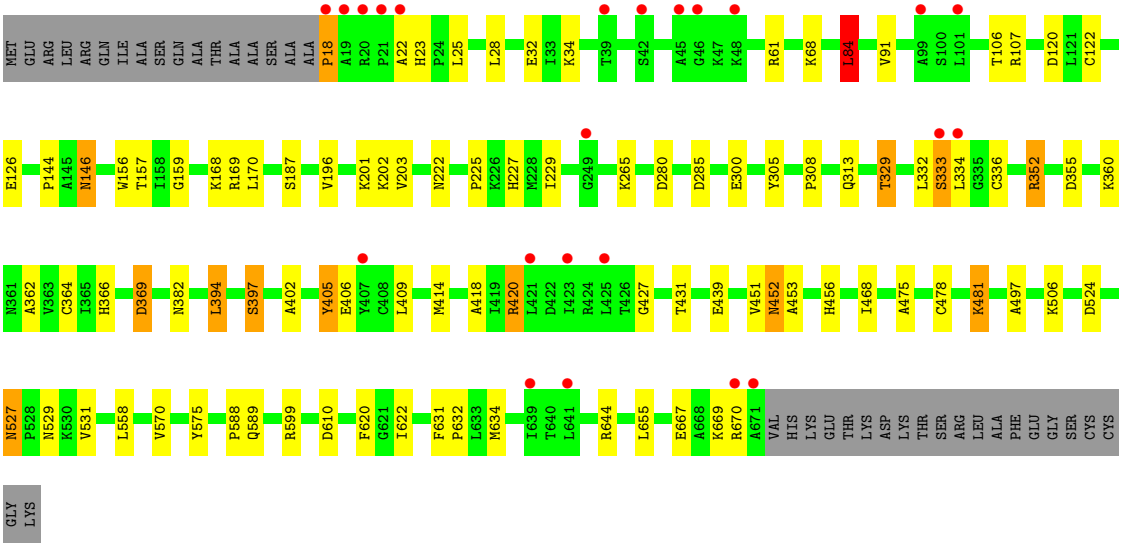
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	527	529	529	0	2
6	B	579	583	583	0	4
6	C	497	499	499	0	2
6	D	462	465	465	0	3
6	E	460	462	462	0	2
6	F	501	503	503	0	2

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.

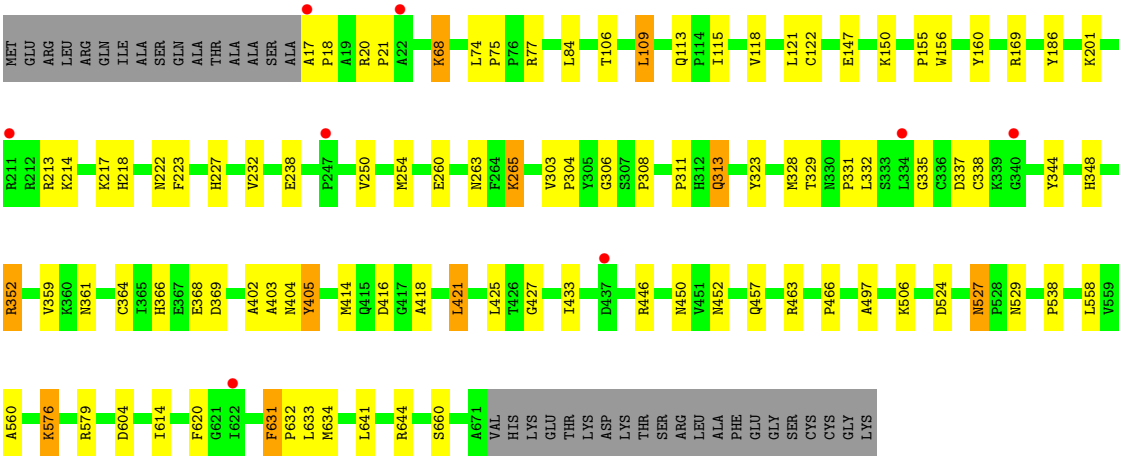
• Molecule 1: Peroxisomal primary amine oxidase

Chain A:



• Molecule 1: Peroxisomal primary amine oxidase

Chain B:



• Molecule 1: Peroxisomal primary amine oxidase

Chain C: 4% 79% 14% • 5%

MET GLU ARG LEU ARG GLN ILE ALA SER GLN ALA THR ALA ALA SER ALA ALA P18 A19 R20 P21 A22 H23 P24 L25 R57 L74 R77 S102 P114 T115 L116 L121 C122 E125 I135 V139 L140 S141 A145 N146 E147 M148 P155 W156 T157 L170

V175 D182 L190 D197 K202 R211 R212 R213 K214 V215 N222 H227 M228 G233 P237 P241 T242 T245 Q246 P247 E248 E260 W261 S262 N263 F264 K265 Y272 I296 M301 I302 V303 Q313 A317 L318 M328 T329 L332 S333 L334 G335

C336 I342 H343 Y344 K360 N361 C364 L373 F374 N382 R390 L394 A402 Y405 M414 A418 I419 R420 I423 R424 I425 I426 G427 G435 D436 D437 R446 N452 Q457 S461 I464 I468 C478 K481 Y485 F498

K506 T507 V508 K509 R521 S522 W523 N527 P528 N529 K530 V531 L543 V544 S557 L558 P564 W565 V570 R579 P588 R599 E600 W601 I602 D610 G621 F631 P632 L633 M634 E637 P638 I639 T640 L641 M642 L643 R644 P645 R646 N652 L655 Q658

P659 S660 Y661 A668 K669 R670 A671 V672 HIS LYS GLU THR LYS ASP LYS THR SER ARG LEU ALA PHE GLU GLY SER CYS CYS GLY LYS

• Molecule 1: Peroxisomal primary amine oxidase

Chain D: 9% 79% 14% • 5%

MET GLU ARG LEU ARG GLN ILE ALA SER GLN ALA THR ALA ALA SER ALA ALA P18 A19 R20 P21 A22 H23 P24 E32 A35 A36 T37 N38 T39 V40 K41 S42 Y43 F44 A45 G46 K47 K48 F51 W67 K68 E69 Q70 R77 L98 S102 L109 V118 L121

C122 E125 E126 V127 N130 D131 P132 I135 E136 L140 S141 G142 I143 N146 E147 M148 P155 Y186 V196 E199 V203 R211 R212 R213 Y224 H227 M228 I229 E230 K231 P240 N243 V244 T245 Q246 P247 E248 G249 V250 T255 M259 F266

Y272 D280 G287 P291 I296 S297 L298 M301 I302 Y305 F310 Q313 A317 L318 D319 Y327 M328 L334 G335 C336 G340 V341 I342 H343 Y344 L345 D351 R352 A353 N361 C364 I365 H366 L394 S397 A402 Y405 E406 Y407 C408

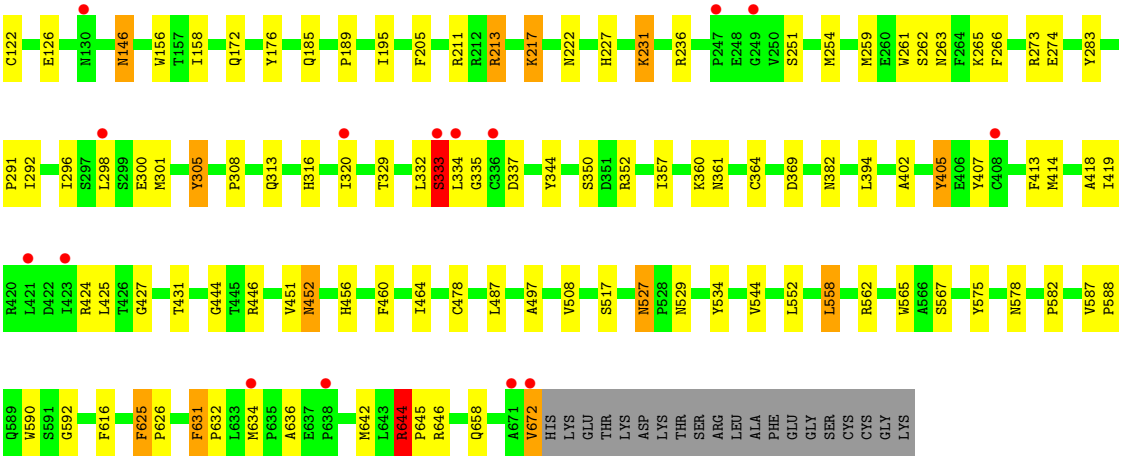
L409 F413 M414 A418 L421 D422 I423 R424 L425 T426 G427 I428 L429 N430 G444 Y448 P449 N452 H456 L459 F460 R463 I464 A480 K481 S482 S483 P484 Y494 R521 D524 N527 P528 N529 V544 L552 A553 K554 L558 Y581 D604

D610 D613 T619 F620 G621 I622 D630 F631 P632 L633 M634 P638 I639 T640 L641 M642 L643 R644 L655 K669 R670 A671 V672 HIS LYS GLU THR LYS ASP LYS THR SER ARG LEU ALA PHE GLU GLY SER CYS CYS GLY LYS

• Molecule 1: Peroxisomal primary amine oxidase

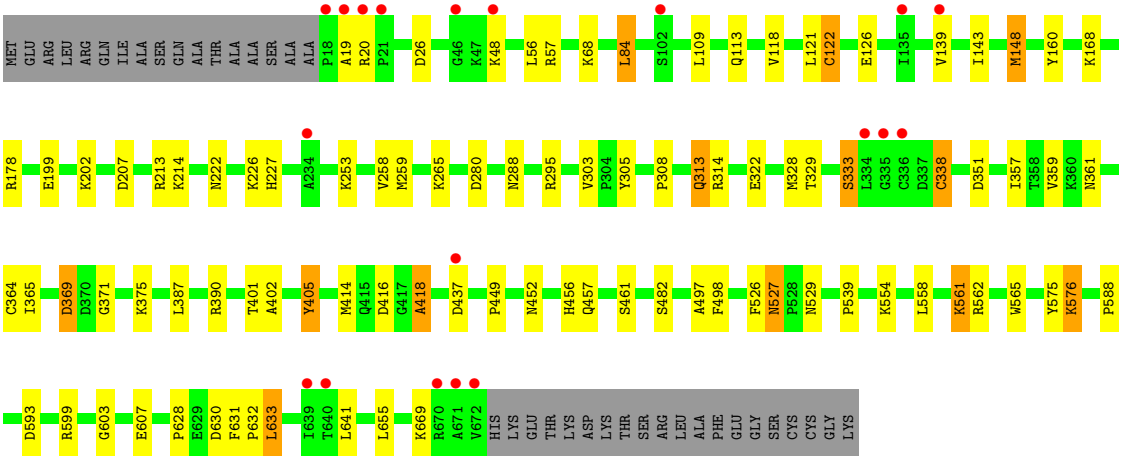
Chain E: 4% 76% 16% • 5%

MET GLU ARG LEU ARG GLN ILE ALA SER GLN ALA THR ALA ALA SER ALA ALA PRO A19 R20 P21 A22 H23 P24 L25 K34 Y43 F44 A45 G46 K47 K48 V54 R57 R61 K68 L74 R77 Y81 E85 K88 V91 S100 L101 P114



- Molecule 1: Peroxisomal primary amine oxidase

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	104.24Å 233.71Å 105.05Å 90.00° 96.57° 90.00°	Depositor
Resolution (Å)	48.90 – 2.25 48.90 – 2.25	Depositor EDS
% Data completeness (in resolution range)	98.8 (48.90-2.25) 98.8 (48.90-2.25)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.40 (at 2.24Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.169 , 0.230 0.168 , 0.228	Depositor DCC
R_{free} test set	11654 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	33.7	Xtriage
Anisotropy	0.193	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 43.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.007 for l,-k,h	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	34660	wwPDB-VP
Average B, all atoms (Å^2)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.39% of the height of the origin peak. No significant pseudotranslation is detected.*

[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: ABN, GOL, TYQ, CU, PEO

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	1.09	6/5395 (0.1%)	0.95	10/7340 (0.1%)
1	B	1.21	8/5387 (0.1%)	1.01	11/7328 (0.2%)
1	C	1.05	2/5396 (0.0%)	0.95	9/7343 (0.1%)
1	D	0.98	1/5382 (0.0%)	0.90	11/7323 (0.2%)
1	E	1.13	11/5418 (0.2%)	0.98	9/7372 (0.1%)
1	F	1.10	7/5386 (0.1%)	0.98	18/7326 (0.2%)
All	All	1.10	35/32364 (0.1%)	0.96	68/44032 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	E	0	1
All	All	0	2

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	478	CYS	CB-SG	9.19	1.97	1.82
1	A	478	CYS	CB-SG	8.77	1.97	1.82
1	B	620	PHE	CE1-CZ	6.48	1.49	1.37
1	B	186	TYR	CD2-CE2	-6.45	1.29	1.39
1	B	560	ALA	CA-CB	6.38	1.65	1.52
1	E	305	TYR	CG-CD1	6.26	1.47	1.39
1	B	232	VAL	CB-CG1	5.98	1.65	1.52
1	A	570	VAL	CB-CG1	5.98	1.65	1.52
1	A	122	CYS	CB-SG	5.88	1.92	1.82
1	E	460	PHE	CE1-CZ	5.78	1.48	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	498	PHE	CE1-CZ	5.76	1.48	1.37
1	E	122	CYS	CB-SG	5.66	1.91	1.82
1	E	631	PHE	CE2-CZ	5.65	1.48	1.37
1	A	620	PHE	CE2-CZ	5.64	1.48	1.37
1	D	482	SER	CB-OG	-5.59	1.34	1.42
1	F	322	GLU	CD-OE1	5.55	1.31	1.25
1	F	561	LYS	CD-CE	5.43	1.64	1.51
1	C	122	CYS	CB-SG	5.37	1.91	1.82
1	A	420	ARG	CB-CG	-5.35	1.38	1.52
1	F	199	GLU	CG-CD	5.35	1.59	1.51
1	B	122	CYS	CB-SG	5.33	1.91	1.82
1	E	300	GLU	CG-CD	5.32	1.59	1.51
1	C	272	TYR	CE1-CZ	5.30	1.45	1.38
1	A	300	GLU	CD-OE1	5.28	1.31	1.25
1	F	418	ALA	CA-CB	5.26	1.63	1.52
1	B	631	PHE	CE2-CZ	5.24	1.47	1.37
1	E	625	PHE	CE1-CZ	5.21	1.47	1.37
1	B	18	PRO	N-CD	5.20	1.55	1.47
1	E	508	VAL	CB-CG2	5.19	1.63	1.52
1	E	126	GLU	CB-CG	5.18	1.61	1.52
1	B	160	TYR	CD2-CE2	5.17	1.47	1.39
1	E	205	PHE	CE1-CZ	5.14	1.47	1.37
1	E	261	TRP	CE3-CZ3	5.06	1.47	1.38
1	F	603	GLY	N-CA	5.06	1.53	1.46
1	F	526	PHE	CD2-CE2	5.01	1.49	1.39

All (68) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	295	ARG	NE-CZ-NH1	9.11	124.85	120.30
1	C	641	LEU	CA-CB-CG	8.63	135.16	115.30
1	E	446	ARG	NE-CZ-NH2	-8.41	116.10	120.30
1	B	463	ARG	NE-CZ-NH2	-8.10	116.25	120.30
1	E	446	ARG	NE-CZ-NH1	7.98	124.29	120.30
1	A	420	ARG	NE-CZ-NH1	-7.87	116.36	120.30
1	E	213	ARG	NE-CZ-NH1	7.49	124.05	120.30
1	F	416	ASP	CB-CG-OD1	7.34	124.91	118.30
1	C	646	ARG	NE-CZ-NH2	-7.33	116.63	120.30
1	D	604	ASP	CB-CG-OD1	7.30	124.87	118.30
1	B	558	LEU	CB-CG-CD1	-7.23	98.72	111.00
1	F	295	ARG	NE-CZ-NH2	-7.04	116.78	120.30
1	E	213	ARG	NE-CZ-NH2	-6.99	116.81	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	562	ARG	NE-CZ-NH1	6.91	123.75	120.30
1	E	236	ARG	NE-CZ-NH2	-6.79	116.91	120.30
1	B	421	LEU	CB-CG-CD2	6.70	122.38	111.00
1	A	394	LEU	CA-CB-CG	6.65	130.59	115.30
1	A	84	LEU	CA-CB-CG	6.61	130.51	115.30
1	B	416	ASP	CB-CG-OD1	6.38	124.04	118.30
1	B	463	ARG	NE-CZ-NH1	6.29	123.44	120.30
1	A	369	ASP	CB-CG-OD1	6.13	123.82	118.30
1	F	178	ARG	NE-CZ-NH2	-6.13	117.24	120.30
1	D	351	ASP	CB-CG-OD1	6.08	123.77	118.30
1	A	285	ASP	CB-CG-OD1	6.05	123.74	118.30
1	F	57	ARG	NE-CZ-NH1	6.05	123.32	120.30
1	F	562	ARG	NE-CZ-NH2	-6.04	117.28	120.30
1	C	182	ASP	CB-CG-OD1	5.95	123.65	118.30
1	C	610	ASP	CB-CG-OD1	5.88	123.60	118.30
1	A	352	ARG	NE-CZ-NH1	5.85	123.23	120.30
1	B	17	ALA	C-N-CD	5.80	140.58	128.40
1	B	109	LEU	CA-CB-CG	5.78	128.60	115.30
1	E	644[A]	ARG	NE-CZ-NH1	5.70	123.15	120.30
1	E	644[B]	ARG	NE-CZ-NH1	5.70	123.15	120.30
1	D	77	ARG	CG-CD-NE	-5.67	99.90	111.80
1	C	420	ARG	NE-CZ-NH1	5.61	123.10	120.30
1	A	610	ASP	CB-CG-OD1	5.61	123.34	118.30
1	A	369	ASP	CB-CG-OD2	-5.60	113.26	118.30
1	F	351	ASP	CB-CG-OD1	5.56	123.30	118.30
1	D	613	ASP	CB-CG-OD1	5.55	123.30	118.30
1	F	57	ARG	NE-CZ-NH2	-5.47	117.56	120.30
1	F	314	ARG	NE-CZ-NH2	-5.46	117.57	120.30
1	C	579	ARG	NE-CZ-NH2	-5.45	117.58	120.30
1	C	57	ARG	NE-CZ-NH2	-5.45	117.58	120.30
1	C	641	LEU	CB-CG-CD2	5.40	120.18	111.00
1	C	446	ARG	NE-CZ-NH2	-5.39	117.61	120.30
1	E	369	ASP	CB-CG-OD2	-5.38	113.46	118.30
1	F	599	ARG	NE-CZ-NH1	-5.38	117.61	120.30
1	F	207	ASP	CB-CG-OD1	5.35	123.12	118.30
1	D	77	ARG	NE-CZ-NH2	-5.31	117.64	120.30
1	B	524	ASP	CB-CG-OD2	-5.30	113.53	118.30
1	F	369	ASP	CB-CG-OD2	-5.28	113.55	118.30
1	D	610	ASP	CB-CG-OD1	5.27	123.05	118.30
1	D	633	LEU	CA-CB-CG	5.24	127.36	115.30
1	B	641	LEU	CB-CG-CD2	-5.21	102.14	111.00
1	D	345	LEU	CA-CB-CG	5.21	127.27	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	416	ASP	CB-CG-OD2	-5.18	113.64	118.30
1	D	604	ASP	CB-CG-OD2	-5.15	113.67	118.30
1	B	254	MET	CG-SD-CE	5.14	108.42	100.20
1	F	84	LEU	CA-CB-CG	5.13	127.10	115.30
1	F	280	ASP	CB-CG-OD1	5.13	122.91	118.30
1	E	352	ARG	NE-CZ-NH1	5.12	122.86	120.30
1	A	394	LEU	CB-CG-CD2	5.11	119.69	111.00
1	D	521	ARG	NE-CZ-NH1	-5.11	117.75	120.30
1	B	446	ARG	NE-CZ-NH1	5.11	122.85	120.30
1	D	463	ARG	NE-CZ-NH2	-5.06	117.77	120.30
1	F	633	LEU	CB-CG-CD2	5.03	119.54	111.00
1	A	599	ARG	NE-CZ-NH2	-5.01	117.80	120.30
1	F	630	ASP	CB-CG-OD1	5.01	122.81	118.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	18	PRO	Peptide
1	E	333	SER	Peptide

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	5227	0	5096	79	0
1	B	5227	0	5086	73	0
1	C	5228	0	5084	84	0
1	D	5223	0	5075	79	0
1	E	5245	0	5127	96	0
1	F	5227	0	5094	56	0
2	A	30	0	40	6	0
2	B	36	0	48	5	0
2	C	36	0	48	4	0
2	D	24	0	32	9	0
2	E	24	0	32	6	0
2	F	30	0	40	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
4	A	2	0	0	1	0
4	B	2	0	0	0	0
4	E	2	0	0	0	0
4	F	2	0	0	1	0
5	A	8	0	9	2	0
5	B	8	0	9	2	0
5	C	8	0	9	5	0
5	D	8	0	9	3	0
5	E	8	0	9	2	0
5	F	8	0	9	3	0
6	A	529	0	0	12	0
6	B	583	0	0	16	0
6	C	499	0	0	13	0
6	D	465	0	0	12	0
6	E	462	0	0	11	0
6	F	503	0	0	8	0
All	All	34660	0	30856	453	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 7.

All (453) 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)
1:E:672:VAL:HG23	6:E:1198:HOH:O	1.40	1.20
6:E:1141:HOH:O	1:F:122[B]:CYS:SG	2.05	1.14
1:D:68:LYS:HE3	2:D:702:GOL:H2	1.38	1.05
1:D:23:HIS:HE2	2:D:702:GOL:H11	1.20	1.04
1:C:638:PRO:HD2	6:D:817[B]:HOH:O	1.59	1.02
1:B:214:LYS:O	2:B:706:GOL:H11	1.60	1.00
1:E:578:ASN:H	2:E:706:GOL:H11	1.27	0.97
1:A:280:ASP:OD2	2:A:703:GOL:H12	1.66	0.96
6:C:1264:HOH:O	1:D:122[A]:CYS:SG	2.22	0.95
1:E:54[B]:VAL:CG2	1:E:350:SER:HB2	1.95	0.95
1:B:348:HIS:HD2	6:B:1180:HOH:O	1.50	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:23:HIS:HD2	1:A:25:LEU:H	1.14	0.93
1:A:332:LEU:O	1:A:333:SER:HB3	1.71	0.89
1:C:23:HIS:HD2	1:C:25:LEU:H	1.17	0.87
1:A:201:LYS:HE2	6:A:1284:HOH:O	1.73	0.87
1:A:168:LYS:HB2	1:A:170[B]:LEU:HD11	1.58	0.85
1:E:23:HIS:HD2	1:E:25:LEU:H	1.22	0.85
1:C:644:ARG:HD2	6:C:1280:HOH:O	1.76	0.85
1:F:148:MET:HE2	1:F:148:MET:HA	1.60	0.83
1:F:405:TYQ:N5	5:F:708:ABN:N	2.28	0.81
1:A:169:ARG:C	1:A:170[B]:LEU:HD12	2.03	0.79
1:B:74:LEU:HD13	1:B:74:LEU:C	2.02	0.78
1:B:218:HIS:HB3	2:B:707:GOL:H12	1.66	0.78
1:A:405:TYQ:N5	5:A:708:ABN:N	2.31	0.78
1:A:427:GLY:O	1:A:634[A]:MET:HG2	1.83	0.78
1:D:527:ASN:HD22	1:D:529:ASN:H	1.30	0.78
1:A:332:LEU:O	1:A:333:SER:CB	2.31	0.78
1:B:348:HIS:CD2	6:B:1180:HOH:O	2.29	0.78
1:C:20:ARG:HD2	1:C:74:LEU:HD21	1.66	0.77
1:A:168:LYS:O	1:A:170[B]:LEU:CD1	2.34	0.76
1:E:578:ASN:H	2:E:706:GOL:C1	1.99	0.76
1:C:121:LEU:HD11	5:C:708:ABN:H4	1.67	0.76
1:C:157[A]:THR:HG22	6:C:911:HOH:O	1.85	0.76
1:E:23:HIS:HE1	2:E:704:GOL:O2	1.68	0.76
1:B:68:LYS:HE3	2:B:704:GOL:H11	1.67	0.75
1:F:148:MET:HA	1:F:148:MET:CE	2.16	0.75
1:E:544:VAL:HG21	1:E:644[B]:ARG:NH2	2.02	0.74
1:D:301:MET:HB3	6:D:1245:HOH:O	1.87	0.74
1:E:333:SER:HA	1:E:335:GLY:N	2.03	0.74
1:C:23:HIS:HE1	2:C:702:GOL:O3	1.69	0.74
1:E:54[B]:VAL:HG22	1:E:350:SER:HB2	1.69	0.73
1:C:344:TYR:CB	1:C:361:ASN:HD22	2.01	0.73
1:D:23:HIS:NE2	2:D:702:GOL:H11	2.01	0.73
2:C:703:GOL:H31	6:C:1152:HOH:O	1.88	0.72
1:F:527:ASN:HD22	1:F:529:ASN:H	1.37	0.72
1:B:425:LEU:HB3	6:B:1296:HOH:O	1.90	0.72
1:E:578:ASN:N	2:E:706:GOL:H11	2.04	0.71
1:B:404:ASN:HD21	1:B:405:TYQ:CZ	2.04	0.71
1:C:527:ASN:C	1:C:527:ASN:HD22	1.93	0.71
1:A:23:HIS:HE1	2:A:703:GOL:O1	1.74	0.70
1:C:328[B]:MET:HE2	6:C:1227:HOH:O	1.91	0.70
1:E:156:TRP:CD1	5:E:707:ABN:H2	2.26	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:156:TRP:CD1	5:B:709:ABN:H2	2.28	0.69
1:A:18:PRO:HG2	1:A:32:GLU:HG2	1.73	0.68
1:E:333:SER:HB2	6:E:1122:HOH:O	1.92	0.68
1:B:644:ARG:HD2	6:B:1375:HOH:O	1.92	0.68
1:E:21:PRO:HG3	1:E:77:ARG:CZ	2.24	0.68
1:A:336:CYS:HB3	6:A:1257:HOH:O	1.93	0.68
1:E:211[A]:ARG:HE	1:E:213:ARG:HD2	1.59	0.67
1:A:157[A]:THR:HG21	1:A:588:PRO:HB3	1.77	0.67
1:C:402:ALA:O	1:C:405:TYQ:HD2	1.94	0.67
1:A:669:LYS:HD3	6:B:1184:HOH:O	1.95	0.66
1:C:23:HIS:CD2	1:C:25:LEU:H	2.08	0.66
1:E:527:ASN:C	1:E:527:ASN:HD22	1.97	0.66
1:C:296:ILE:HD12	1:C:464:ILE:HG12	1.78	0.66
1:C:427:GLY:O	1:C:634[A]:MET:HG2	1.96	0.66
1:C:125:GLU:HB2	6:C:1266:HOH:O	1.95	0.66
1:E:54[B]:VAL:HG22	1:E:350:SER:CB	2.26	0.66
1:A:170[B]:LEU:HD13	1:A:589:GLN:HE22	1.61	0.65
1:C:637:GLU:HG2	6:D:817[B]:HOH:O	1.95	0.65
1:D:51:PHE:HD2	6:D:1247:HOH:O	1.78	0.65
1:F:68:LYS:HE3	2:F:702:GOL:H2	1.77	0.65
1:A:644:ARG:HD2	6:A:1259:HOH:O	1.96	0.65
1:B:331:PRO:HD2	6:B:1308:HOH:O	1.97	0.64
1:E:158:ILE:HA	1:E:172:GLN:HG2	1.78	0.64
1:E:544:VAL:HG21	1:E:644[B]:ARG:HH21	1.61	0.64
1:E:427:GLY:O	1:E:634[C]:MET:HG2	1.97	0.64
1:C:21:PRO:HG3	1:C:77:ARG:CZ	2.28	0.64
1:C:527:ASN:HD22	1:C:529:ASN:H	1.46	0.64
1:E:68:LYS:HE3	2:E:704:GOL:H32	1.80	0.63
1:B:527:ASN:HD21	1:B:529:ASN:HD22	1.47	0.63
1:C:527:ASN:HD21	1:C:529:ASN:HD22	1.44	0.63
1:E:54[B]:VAL:HG23	1:E:350:SER:HB2	1.78	0.63
1:C:527:ASN:ND2	1:C:529:ASN:H	1.97	0.63
1:A:168:LYS:O	1:A:170[B]:LEU:HD13	1.98	0.62
1:C:222:ASN:HB3	1:C:227:HIS:CG	2.33	0.62
1:C:527:ASN:ND2	1:C:529:ASN:HD22	1.98	0.62
1:A:352:ARG:HD2	6:A:1269:HOH:O	1.99	0.62
1:D:343:HIS:HB2	2:D:705:GOL:H2	1.81	0.62
1:F:402:ALA:HB1	5:F:708:ABN:H6	1.82	0.61
1:F:527:ASN:HD21	1:F:529:ASN:HB2	1.66	0.61
1:C:116:LEU:CD1	1:C:157[A]:THR:HG23	2.30	0.61
1:A:23:HIS:CE1	2:A:703:GOL:O1	2.54	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:414:MET:HE3	1:B:418:ALA:HB3	1.81	0.61
1:A:414:MET:HE3	1:A:418:ALA:HB3	1.82	0.60
1:D:68:LYS:CE	2:D:702:GOL:H2	2.25	0.60
1:E:631:PHE:CG	1:E:632:PRO:HA	2.36	0.60
1:A:157[A]:THR:HG22	1:A:159:GLY:H	1.66	0.60
1:B:121:LEU:HD12	1:B:328[B]:MET:HE3	1.83	0.60
1:E:631:PHE:CD1	1:E:632:PRO:HA	2.37	0.60
1:A:168:LYS:HE3	6:A:1276:HOH:O	2.01	0.60
1:C:344:TYR:CD1	1:C:361:ASN:HB3	2.36	0.60
1:E:527:ASN:HD21	1:E:529:ASN:HD22	1.49	0.59
1:B:147:GLU:HB3	1:B:150:LYS:HD3	1.83	0.59
1:B:250:VAL:HG22	6:B:959:HOH:O	2.02	0.59
1:D:527:ASN:ND2	1:D:529:ASN:H	1.99	0.59
1:F:313:GLN:H	1:F:313:GLN:HE21	1.50	0.59
1:D:140:LEU:HD22	6:D:1221:HOH:O	2.00	0.59
1:B:527:ASN:HD22	1:B:529:ASN:H	1.49	0.59
2:C:707:GOL:H12	6:C:919:HOH:O	2.03	0.59
1:D:70:GLN:HG2	6:D:1207:HOH:O	2.01	0.59
1:A:202:LYS:HD2	6:A:1311:HOH:O	2.03	0.58
1:D:344:TYR:HB3	1:D:361:ASN:HD22	1.67	0.58
1:A:631:PHE:CD1	1:A:632:PRO:HA	2.38	0.58
1:F:265:LYS:HE3	2:F:702:GOL:O2	2.03	0.58
1:B:121:LEU:CD1	1:B:328[B]:MET:HE3	2.33	0.58
1:D:642:MET:HE3	1:D:644[B]:ARG:NH1	2.19	0.58
1:E:425:LEU:HB3	6:E:1146:HOH:O	2.02	0.58
1:A:397[A]:SER:HB2	1:A:409:LEU:O	2.03	0.57
1:B:402:ALA:O	1:B:405:TYQ:HD2	2.03	0.57
1:D:37:THR:HG22	1:D:51:PHE:CE1	2.39	0.57
1:B:20:ARG:CZ	1:B:74:LEU:HD11	2.34	0.57
1:B:538:PRO:HG3	6:B:1114:HOH:O	2.05	0.57
1:C:175:VAL:HG11	1:C:190:LEU:HD12	1.84	0.57
1:E:301:MET:HG3	1:E:320:ILE:HD12	1.84	0.57
1:B:527:ASN:ND2	1:B:529:ASN:HD22	2.02	0.57
1:F:405:TYQ:OZ	4:F:707:PEO:O2	2.23	0.56
1:A:527:ASN:HD22	1:A:529:ASN:H	1.53	0.56
1:A:481[A]:LYS:HB3	1:A:481[A]:LYS:HZ3	1.70	0.56
1:A:527:ASN:HD22	1:A:527:ASN:C	2.08	0.56
1:B:631:PHE:CG	1:B:632:PRO:HA	2.41	0.56
1:A:634[A]:MET:HE1	6:A:1256:HOH:O	2.04	0.56
1:B:218:HIS:HD2	1:B:450:ASN:HD22	1.52	0.56
1:D:342:ILE:HG21	1:D:344:TYR:CZ	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:527:ASN:HD22	1:E:529:ASN:H	1.52	0.56
1:B:576[A]:LYS:HE2	1:B:579:ARG:NH2	2.20	0.56
1:A:146:ASN:H	1:A:146:ASN:HD22	1.54	0.56
1:E:414:MET:HE3	1:E:418:ALA:HB3	1.88	0.56
1:C:652:ASN:HB3	1:C:655:LEU:HD11	1.88	0.56
1:E:91:VAL:HG11	1:E:114:PRO:HG3	1.88	0.56
1:A:366:HIS:HD2	6:A:1300:HOH:O	1.89	0.55
1:E:497:ALA:HB2	1:F:308:PRO:HB3	1.89	0.55
1:B:427:GLY:O	1:B:634:MET:HG2	2.06	0.55
1:E:21:PRO:HB3	6:E:1209:HOH:O	2.06	0.55
1:E:283:TYR:HB2	1:E:292:ILE:HD11	1.88	0.55
1:A:157[A]:THR:HG23	6:A:968:HOH:O	2.07	0.54
1:D:23:HIS:HE2	2:D:702:GOL:C1	2.07	0.54
1:E:333:SER:HA	1:E:334:LEU:C	2.28	0.54
1:E:407:TYR:CD1	1:E:425:LEU:HD22	2.42	0.54
1:D:405:TYQ:N5	5:D:706:ABN:N	2.55	0.54
1:A:631:PHE:CG	1:A:632:PRO:HA	2.43	0.54
1:E:527:ASN:ND2	1:E:529:ASN:H	2.05	0.54
1:A:23:HIS:CD2	1:A:25:LEU:H	2.06	0.54
1:E:158:ILE:HD12	1:E:195:ILE:HG23	1.90	0.54
1:A:527:ASN:HD21	1:A:529:ASN:HD22	1.55	0.54
1:A:106:THR:O	1:A:107:ARG:HB3	2.08	0.54
1:A:201:LYS:CE	6:A:1284:HOH:O	2.44	0.54
1:F:259:MET:CE	1:F:365:ILE:HG21	2.38	0.54
1:A:265:LYS:HD3	2:A:703:GOL:H32	1.88	0.54
1:D:402:ALA:HB1	5:D:706:ABN:H6	1.89	0.54
1:F:461:SER:HB2	1:F:565:TRP:CE3	2.43	0.54
1:E:91:VAL:CG1	1:E:114:PRO:HG3	2.37	0.53
1:C:23:HIS:CE1	2:C:702:GOL:O3	2.55	0.53
1:E:296:ILE:HD12	1:E:464:ILE:HG12	1.89	0.53
1:C:20:ARG:HD2	1:C:74:LEU:CD2	2.36	0.53
1:C:116:LEU:HD12	1:C:157[A]:THR:HG23	1.89	0.53
1:C:175:VAL:CG1	1:C:190:LEU:HD12	2.37	0.53
1:F:631:PHE:CG	1:F:632:PRO:HA	2.43	0.53
1:B:260:GLU:HG2	1:B:265:LYS:HG3	1.90	0.53
1:F:222:ASN:HB3	1:F:227:HIS:CG	2.43	0.53
1:C:509:LYS:NZ	6:C:1167:HOH:O	2.42	0.53
1:A:669:LYS:CD	6:B:1184:HOH:O	2.56	0.53
1:A:655:LEU:HD22	1:B:223:PHE:HB2	1.91	0.53
1:F:527:ASN:ND2	1:F:529:ASN:H	2.05	0.52
2:F:704:GOL:H11	6:F:1256:HOH:O	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:564:PRO:HG3	1:C:599:ARG:NH2	2.25	0.52
1:D:342:ILE:HG23	1:D:364[B]:CYS:SG	2.49	0.52
1:F:575:TYR:O	1:F:576[B]:LYS:HD3	2.10	0.52
1:A:667:GLU:HG2	1:A:670:ARG:NH2	2.25	0.52
1:B:506:LYS:NZ	6:B:1173:HOH:O	2.42	0.52
1:D:630:ASP:HB3	1:D:634:MET:HG3	1.92	0.52
1:C:145:ALA:O	1:C:148:MET:HG2	2.10	0.52
1:C:260:GLU:HG2	1:C:265:LYS:HG3	1.92	0.52
1:C:332:LEU:O	1:C:333:SER:CB	2.58	0.52
1:C:631:PHE:CD1	1:C:632:PRO:HA	2.45	0.52
1:A:144:PRO:HB2	1:A:146:ASN:ND2	2.26	0.51
1:C:262:SER:O	1:C:263:ASN:HB2	2.10	0.51
1:F:333:SER:HB3	1:F:361:ASN:OD1	2.11	0.51
1:F:160:TYR:CD2	1:F:558:LEU:HD11	2.46	0.51
1:A:68:LYS:HE3	2:A:703:GOL:H31	1.91	0.51
1:D:527:ASN:HD21	1:D:529:ASN:HB2	1.76	0.51
1:C:425:LEU:HD23	6:C:1235:HOH:O	2.10	0.51
1:D:554:LYS:HE3	6:D:1168:HOH:O	2.10	0.51
1:B:113:GLN:OE1	1:B:169:ARG:HG3	2.11	0.50
1:B:527:ASN:ND2	1:B:529:ASN:H	2.10	0.50
1:A:402:ALA:O	1:A:405:TYQ:HD2	2.11	0.50
1:D:310:PHE:HA	1:D:313:GLN:HE22	1.76	0.50
1:E:402:ALA:O	1:E:405:TYQ:HD2	2.12	0.50
1:E:444:GLY:HA3	1:E:452:ASN:HD21	1.75	0.50
1:F:168:LYS:CE	6:F:1042:HOH:O	2.60	0.50
1:E:464:ILE:HB	1:E:616:PHE:HB3	1.94	0.50
1:B:121:LEU:O	1:B:155:PRO:HG3	2.11	0.50
1:D:231:LYS:HE2	6:D:1223:HOH:O	2.11	0.50
1:B:222:ASN:HB3	1:B:227:HIS:ND1	2.27	0.50
1:D:524:ASP:OD2	6:D:900:HOH:O	2.20	0.50
1:D:394:LEU:HB3	1:D:413:PHE:HB2	1.94	0.49
1:D:631:PHE:CG	1:D:632:PRO:HA	2.47	0.49
1:F:26:ASP:O	1:F:56:LEU:HD22	2.11	0.49
1:B:214:LYS:O	2:B:706:GOL:C1	2.48	0.49
1:D:296:ILE:HD12	1:D:464:ILE:HG12	1.94	0.49
1:E:176:TYR:CE1	1:E:189:PRO:HB3	2.46	0.49
1:E:344:TYR:HB3	1:E:361:ASN:HD22	1.77	0.49
1:A:481[A]:LYS:HB3	1:A:481[A]:LYS:NZ	2.27	0.49
1:B:115:ILE:HD11	1:B:323:TYR:C	2.32	0.49
1:C:135:ILE:HG12	1:C:148:MET:HG3	1.94	0.49
1:C:157[A]:THR:HG21	1:C:588:PRO:HB3	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:211[A]:ARG:HE	1:E:213:ARG:CD	2.25	0.49
1:D:414:MET:HE3	1:D:418:ALA:HB3	1.95	0.49
1:F:148:MET:CE	1:F:148:MET:CA	2.90	0.49
1:F:168:LYS:HE3	6:F:1042:HOH:O	2.11	0.49
1:A:157[A]:THR:CG2	1:A:588:PRO:HB3	2.42	0.49
1:B:218:HIS:CD2	1:B:450:ASN:HD22	2.30	0.49
1:B:222:ASN:HB3	1:B:227:HIS:CG	2.46	0.49
1:C:402:ALA:HB1	5:C:708:ABN:H6	1.95	0.49
1:B:631:PHE:CD1	1:B:632:PRO:HA	2.48	0.49
1:E:425:LEU:O	1:E:636:ALA:HA	2.13	0.49
1:F:313:GLN:H	1:F:313:GLN:NE2	2.11	0.49
1:E:405:TYQ:N5	5:E:707:ABN:N	2.61	0.49
1:B:74:LEU:C	1:B:74:LEU:CD1	2.79	0.48
1:B:338:CYS:SG	1:B:364[B]:CYS:CB	3.01	0.48
1:D:581:TYR:HB3	6:D:984:HOH:O	2.13	0.48
1:D:484:PRO:HD2	2:D:704:GOL:H2	1.95	0.48
1:C:301:MET:O	1:C:318:LEU:HA	2.13	0.48
1:C:631:PHE:CG	1:C:632:PRO:HA	2.48	0.48
1:E:54[B]:VAL:HG12	1:E:81:TYR:HB3	1.95	0.48
1:A:329:THR:HG21	1:A:362:ALA:HB1	1.95	0.48
1:B:466:PRO:HD2	1:B:614:ILE:O	2.13	0.48
1:D:480:ALA:O	1:D:481[A]:LYS:HG2	2.14	0.48
1:F:265:LYS:NZ	2:F:702:GOL:H12	2.29	0.48
1:B:74:LEU:HD13	1:B:75:PRO:N	2.28	0.48
1:E:211[A]:ARG:HG3	1:E:213:ARG:HD2	1.96	0.48
1:B:311:PRO:HA	1:B:313:GLN:HE22	1.78	0.48
1:B:527:ASN:HD22	1:B:527:ASN:C	2.15	0.48
1:C:414:MET:HE3	1:C:418:ALA:HB3	1.95	0.48
1:D:344:TYR:CB	1:D:361:ASN:HD22	2.26	0.48
1:E:23:HIS:CD2	1:E:25:LEU:H	2.14	0.48
1:A:34:LYS:NZ	1:A:355:ASP:OD1	2.47	0.47
1:A:497:ALA:HB2	1:B:308:PRO:HB3	1.96	0.47
1:C:121:LEU:CD1	5:C:708:ABN:H4	2.41	0.47
1:E:632:PRO:HD2	1:F:655:LEU:HD11	1.95	0.47
1:C:506:LYS:HE2	6:C:1073:HOH:O	2.14	0.47
1:D:301:MET:CB	6:D:1245:HOH:O	2.55	0.47
1:E:565:TRP:CD1	1:E:582:PRO:HB2	2.49	0.47
1:B:20:ARG:NH2	1:B:74:LEU:HD11	2.29	0.47
1:D:143:ILE:O	1:D:143:ILE:HG13	2.15	0.47
1:A:120:ASP:OD1	1:A:352:ARG:NH2	2.39	0.47
1:A:527:ASN:ND2	1:A:529:ASN:H	2.12	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:305:TYR:CD2	1:A:456:HIS:HB3	2.50	0.47
1:E:23:HIS:CD2	1:E:24:PRO:HD2	2.49	0.47
1:F:214:LYS:O	2:F:705:GOL:O3	2.18	0.47
1:E:552:LEU:O	1:F:482:SER:OG	2.32	0.47
1:F:641:LEU:C	1:F:641:LEU:HD12	2.35	0.47
1:A:431:THR:HB	1:A:451:VAL:HG13	1.96	0.47
1:F:121:LEU:HD13	6:F:1244:HOH:O	2.15	0.47
1:C:156:TRP:CD1	5:C:708:ABN:H2	2.50	0.47
1:C:405:TYQ:N5	5:C:708:ABN:N	2.62	0.47
1:D:444:GLY:HA3	1:D:452:ASN:HD21	1.79	0.47
1:D:364[B]:CYS:SG	1:D:365:ILE:N	2.88	0.47
1:E:424:ARG:HB3	1:E:636:ALA:HB1	1.96	0.47
1:E:658:GLN:NE2	6:E:1006:HOH:O	2.25	0.47
1:B:344:TYR:CD1	1:B:361:ASN:HB3	2.50	0.46
1:D:20:ARG:HE	1:D:20:ARG:HB3	1.47	0.46
1:A:225:PRO:O	1:A:229:ILE:HG13	2.15	0.46
1:D:196:VAL:HG22	1:D:203:VAL:HG22	1.96	0.46
1:A:222:ASN:HB3	1:A:227:HIS:CG	2.51	0.46
1:F:305:TYR:CD2	1:F:456:HIS:HB3	2.50	0.46
1:D:199:GLU:OE2	1:D:352:ARG:NH2	2.49	0.46
1:D:224:TYR:HB2	1:D:227:HIS:ND1	2.31	0.46
1:E:316:HIS:CE1	1:E:558:LEU:HD13	2.51	0.46
1:E:645:PRO:O	1:E:646:ARG:HD2	2.16	0.46
1:A:170[B]:LEU:HD13	1:A:589:GLN:NE2	2.29	0.46
1:A:667:GLU:HG2	1:A:670:ARG:HH22	1.80	0.46
1:B:121:LEU:HD11	1:B:328[B]:MET:CE	2.45	0.46
1:B:402:ALA:O	1:B:403:ALA:HB3	2.15	0.46
1:E:231:LYS:HD2	6:E:1138:HOH:O	2.16	0.46
1:A:196:VAL:HG22	1:A:203:VAL:HG22	1.98	0.46
1:C:507:THR:O	1:C:508:VAL:C	2.53	0.46
1:F:338:CYS:CB	1:F:364[B]:CYS:SG	3.03	0.46
1:B:328[B]:MET:HE1	6:B:1149:HOH:O	2.16	0.46
1:A:405:TYQ:OZ	4:A:707:PEO:O2	2.33	0.46
1:C:652:ASN:HB3	1:C:655:LEU:CD1	2.46	0.46
1:E:20:ARG:NH1	1:E:74:LEU:HD21	2.31	0.46
1:E:61:ARG:HD2	1:E:575:TYR:CE1	2.51	0.46
1:C:390:ARG:HG3	1:C:660:SER:OG	2.15	0.45
1:D:121:LEU:CD1	1:D:155:PRO:O	2.63	0.45
1:E:407:TYR:CE1	1:E:425:LEU:HD22	2.51	0.45
1:F:669[B]:LYS:HE2	1:F:669[B]:LYS:HB3	1.66	0.45
1:D:121:LEU:HD12	1:D:155:PRO:HG2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:54[B]:VAL:CG2	1:E:350:SER:CB	2.77	0.45
1:E:337:ASP:N	6:E:1122:HOH:O	2.50	0.45
1:C:481:LYS:HE3	6:C:1297:HOH:O	2.15	0.45
1:C:485:TYR:O	1:D:554:LYS:HE2	2.16	0.45
1:E:544:VAL:HG11	1:E:644[B]:ARG:NH2	2.32	0.45
1:F:527:ASN:HD21	1:F:529:ASN:HD22	1.63	0.45
6:B:1193:HOH:O	1:E:487:LEU:HD21	2.15	0.45
1:D:68:LYS:HE3	2:D:702:GOL:C2	2.26	0.45
1:B:303:VAL:HA	1:B:457:GLN:O	2.16	0.45
1:C:342:ILE:HG21	1:C:344:TYR:CZ	2.52	0.45
1:F:371:GLY:HA2	1:F:390:ARG:NH2	2.31	0.45
1:D:280:ASP:OD2	2:D:702:GOL:H12	2.16	0.45
1:F:607:GLU:OE1	6:F:1007:HOH:O	2.21	0.45
1:E:332:LEU:O	1:E:333:SER:O	2.34	0.45
1:C:557:SER:HB2	1:D:494:TYR:O	2.17	0.45
1:E:413:PHE:CE2	1:E:419:ILE:HD13	2.51	0.45
2:B:703:GOL:H32	6:B:1232:HOH:O	2.16	0.44
1:C:141:SER:O	1:C:215:VAL:HG12	2.18	0.44
1:E:333:SER:CB	6:E:1121:HOH:O	2.65	0.44
1:A:61:ARG:HD2	1:A:575:TYR:CE1	2.52	0.44
1:B:218:HIS:CD2	1:B:450:ASN:ND2	2.86	0.44
1:C:303:VAL:HA	1:C:457:GLN:O	2.17	0.44
6:E:937:HOH:O	1:F:118:VAL:HG11	2.17	0.44
1:D:211:ARG:NH1	1:D:213:ARG:HG3	2.32	0.44
1:D:669:LYS:HB3	1:D:669:LYS:HE2	1.84	0.44
1:A:420:ARG:NH1	6:A:1114:HOH:O	2.39	0.44
1:B:20:ARG:NH1	1:B:74:LEU:HD11	2.33	0.44
1:A:168:LYS:C	1:A:170[B]:LEU:CD1	2.85	0.44
1:E:146:ASN:N	1:E:146:ASN:HD22	2.14	0.44
1:E:217:LYS:HA	1:E:217:LYS:HD2	1.76	0.44
1:F:328[B]:MET:HB3	1:F:401:THR:O	2.17	0.44
1:C:638:PRO:CD	1:D:644[B]:ARG:HH22	2.30	0.44
1:D:527:ASN:HD21	1:D:529:ASN:HD22	1.66	0.44
1:F:19:ALA:HB3	6:F:1227:HOH:O	2.18	0.44
1:B:313:GLN:H	1:B:313:GLN:HE21	1.66	0.44
1:C:228:MET:HG3	1:D:655:LEU:O	2.17	0.44
1:E:558:LEU:O	1:E:562:ARG:HG3	2.18	0.44
1:C:170:LEU:HD23	1:C:197:ASP:HA	2.00	0.43
1:F:527:ASN:HB3	1:F:539:PRO:HG2	2.00	0.43
1:B:433:ILE:HD13	1:B:433:ILE:HG21	1.83	0.43
1:B:604:ASP:C	1:B:604:ASP:OD1	2.55	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:272:TYR:HB2	1:D:327:TYR:CE1	2.53	0.43
1:D:305:TYR:CD2	1:D:456:HIS:HB3	2.53	0.43
1:E:265:LYS:CE	2:E:704:GOL:H12	2.49	0.43
1:F:414:MET:HE3	1:F:418:ALA:HB3	2.01	0.43
1:C:637:GLU:HG3	1:D:644[A]:ARG:NH2	2.34	0.43
1:F:561:LYS:NZ	1:F:593:ASP:OD1	2.45	0.43
1:B:338:CYS:CB	1:B:364[B]:CYS:SG	3.06	0.43
1:D:259:MET:HG2	1:D:266:PHE:CZ	2.54	0.43
1:E:644[B]:ARG:HG2	1:E:646:ARG:HD3	2.01	0.43
1:C:452:ASN:C	1:C:452:ASN:HD22	2.22	0.43
1:A:23:HIS:HE1	2:A:703:GOL:C1	2.31	0.43
1:C:211:ARG:NH2	1:C:435:GLY:HA3	2.33	0.43
1:D:407:TYR:CD1	1:D:425:LEU:HD22	2.54	0.43
1:D:527:ASN:HD22	1:D:527:ASN:C	2.21	0.43
1:F:402:ALA:HB1	5:F:708:ABN:C6	2.49	0.43
1:C:481:LYS:CE	6:C:1297:HOH:O	2.67	0.43
1:C:579:ARG:HG2	1:C:601:TRP:CE2	2.54	0.43
1:C:661:TYR:CZ	1:D:334:LEU:HD23	2.54	0.43
1:D:402:ALA:O	1:D:405:TYQ:HD2	2.18	0.43
1:E:23:HIS:HA	1:E:24:PRO:HD3	1.86	0.43
1:F:258:VAL:HG11	2:F:702:GOL:H11	2.01	0.43
1:A:497:ALA:HA	1:B:306:GLY:O	2.19	0.42
1:B:338:CYS:HB3	1:B:364[B]:CYS:SG	2.58	0.42
1:C:523:TRP:CE2	1:C:570:VAL:HG21	2.55	0.42
1:D:344:TYR:CB	1:D:361:ASN:ND2	2.81	0.42
1:E:54[B]:VAL:HG12	1:E:81:TYR:CB	2.49	0.42
1:E:222:ASN:HB3	1:E:227:HIS:CG	2.54	0.42
1:C:402:ALA:HB3	1:C:405:TYQ:HD2	2.01	0.42
1:A:156:TRP:CD1	5:A:708:ABN:H6	2.55	0.42
1:B:20:ARG:NH2	6:B:985:HOH:O	2.51	0.42
1:D:364[B]:CYS:SG	1:D:366:HIS:CD2	3.13	0.42
1:E:308:PRO:HB3	1:F:497:ALA:HB2	2.00	0.42
1:D:291:PRO:HB3	6:D:929:HOH:O	2.18	0.42
1:A:308:PRO:HB3	1:B:497:ALA:HB2	2.01	0.42
1:B:366:HIS:CE1	1:B:368:GLU:CG	3.02	0.42
1:D:402:ALA:HB1	5:D:706:ABN:C6	2.49	0.42
1:A:28:LEU:HD23	1:A:28:LEU:HA	1.87	0.42
1:A:506[A]:LYS:HE2	6:A:1210:HOH:O	2.19	0.42
1:A:634[B]:MET:HE2	1:A:634[B]:MET:HB2	1.86	0.42
1:B:118:VAL:HG23	6:B:1305:HOH:O	2.19	0.42
1:B:156:TRP:CG	5:B:709:ABN:H2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:366:HIS:HE1	1:B:368:GLU:CD	2.23	0.42
1:C:461:SER:HB2	1:C:565:TRP:CE3	2.54	0.42
1:C:498:PHE:CD2	1:D:552:LEU:HD13	2.55	0.42
1:B:304:PRO:HD2	1:B:457:GLN:O	2.19	0.42
1:D:344:TYR:CD1	1:D:361:ASN:HB3	2.55	0.42
1:D:448:TYR:O	1:D:449:PRO:C	2.57	0.42
1:F:402:ALA:O	1:F:405:TYQ:HD2	2.19	0.42
1:A:452:ASN:HD22	1:A:453:ALA:N	2.18	0.42
1:B:352:ARG:HH11	1:B:352:ARG:HB2	1.84	0.42
1:F:139:VAL:HA	1:F:143:ILE:O	2.20	0.42
1:A:414:MET:CE	1:A:418:ALA:HB3	2.48	0.42
1:A:452:ASN:HD22	1:A:452:ASN:C	2.22	0.42
1:D:32:GLU:HG2	1:D:98:LEU:HD13	2.02	0.42
1:E:587:VAL:O	1:E:588:PRO:C	2.58	0.42
1:F:338:CYS:HB3	1:F:364[B]:CYS:SG	2.59	0.42
1:F:527:ASN:ND2	1:F:529:ASN:HB2	2.33	0.42
1:C:670:ARG:O	1:C:670:ARG:HG3	2.20	0.41
1:E:222:ASN:HB3	1:E:227:HIS:ND1	2.34	0.41
1:E:274:GLU:HG2	1:E:298:LEU:O	2.20	0.41
1:F:303:VAL:HG13	1:F:457:GLN:O	2.19	0.41
1:F:437:ASP:HB2	6:F:980:HOH:O	2.20	0.41
1:C:373:LEU:HG	1:C:374:PHE:CD2	2.55	0.41
1:C:527:ASN:C	1:C:527:ASN:ND2	2.67	0.41
1:D:23:HIS:HA	1:D:24:PRO:HD3	1.83	0.41
1:E:634[C]:MET:HE2	1:E:634[C]:MET:HB2	1.84	0.41
1:C:508:VAL:HG11	1:C:602:ILE:HA	2.02	0.41
1:F:113:GLN:O	1:F:588:PRO:HD2	2.20	0.41
1:C:317:ALA:HA	6:C:1148:HOH:O	2.20	0.41
1:C:478:CYS:O	1:C:521:ARG:HA	2.20	0.41
1:E:305:TYR:CD2	1:E:456:HIS:HB3	2.55	0.41
1:C:344:TYR:CG	1:C:361:ASN:ND2	2.77	0.41
1:D:423:ILE:HG22	1:D:425:LEU:HD23	2.01	0.41
1:E:85:GLU:HB3	1:E:88:LYS:HG3	2.01	0.41
1:D:319:ASP:HB3	1:D:328:MET:HE1	2.01	0.41
1:E:527:ASN:ND2	1:E:529:ASN:HD22	2.17	0.41
1:E:590:TRP:CE2	1:E:592:GLY:HA2	2.55	0.41
1:F:527:ASN:HD22	1:F:527:ASN:C	2.24	0.41
1:C:333:SER:HB2	1:C:344:TYR:OH	2.21	0.41
1:C:634[C]:MET:CE	1:C:637:GLU:HB2	2.50	0.41
1:B:121:LEU:CD1	1:B:328[B]:MET:CE	2.98	0.41
1:E:262:SER:O	1:E:263:ASN:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:431:THR:HB	1:E:451:VAL:HG13	2.03	0.41
1:A:84:LEU:HD22	1:A:91:VAL:HG12	2.02	0.41
1:A:336:CYS:HB2	1:B:660:SER:HB3	2.02	0.41
1:B:68:LYS:HG2	6:B:1137:HOH:O	2.19	0.41
1:C:313:GLN:H	1:C:313:GLN:NE2	2.19	0.41
1:E:259:MET:HG2	1:E:266:PHE:CZ	2.56	0.41
1:E:357:ILE:HD12	6:F:1236:HOH:O	2.21	0.41
1:E:534:TYR:CD1	1:F:449:PRO:HD3	2.56	0.41
1:F:375:LYS:HA	1:F:387:LEU:O	2.21	0.41
1:A:468:ILE:O	1:A:527:ASN:HB2	2.21	0.41
1:D:186:TYR:CD2	1:D:428:ILE:HG21	2.56	0.41
1:E:273:ARG:O	1:E:320:ILE:HG23	2.20	0.41
1:A:475:ALA:HA	1:A:524:ASP:O	2.21	0.40
1:B:335:GLY:HA3	1:B:337:ASP:OD1	2.21	0.40
1:C:313:GLN:H	1:C:313:GLN:HE21	1.69	0.40
1:D:211:ARG:HD3	1:D:213:ARG:NE	2.37	0.40
1:D:460:PHE:O	1:D:619:THR:HA	2.21	0.40
1:E:176:TYR:HB3	1:E:185:GLN:HB2	2.02	0.40
1:D:135:ILE:HG12	1:D:148:MET:HG3	2.03	0.40
1:D:302:ILE:HA	1:D:317:ALA:O	2.21	0.40
1:D:631:PHE:CD1	1:D:632:PRO:HA	2.56	0.40
1:E:625:PHE:HA	1:E:626:PRO:HD3	1.87	0.40
1:C:23:HIS:HD2	1:C:25:LEU:N	1.99	0.40
1:E:61:ARG:HD2	1:E:575:TYR:CZ	2.56	0.40
1:E:644[A]:ARG:NH2	6:E:1022:HOH:O	2.54	0.40
1:C:660:SER:HB3	1:D:336:CYS:HB2	2.03	0.40
1:B:21:PRO:HG3	1:B:77:ARG:CZ	2.52	0.40
1:E:34:LYS:HD3	1:E:34:LYS:HA	1.78	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	662/692 (96%)	635 (96%)	25 (4%)	2 (0%)	41	46
1	B	660/692 (95%)	631 (96%)	29 (4%)	0	100	100
1	C	663/692 (96%)	634 (96%)	25 (4%)	4 (1%)	25	25
1	D	660/692 (95%)	633 (96%)	27 (4%)	0	100	100
1	E	664/692 (96%)	637 (96%)	26 (4%)	1 (0%)	47	55
1	F	660/692 (95%)	629 (95%)	30 (4%)	1 (0%)	47	55
All	All	3969/4152 (96%)	3799 (96%)	162 (4%)	8 (0%)	47	55

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	333	SER
1	E	333	SER
1	F	333	SER
1	A	22	ALA
1	C	333	SER
1	C	155	PRO
1	C	114	PRO
1	C	468	ILE

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	574/593 (97%)	550 (96%)	24 (4%)	30	34
1	B	572/593 (96%)	551 (96%)	21 (4%)	34	40
1	C	574/593 (97%)	550 (96%)	24 (4%)	30	34
1	D	572/593 (96%)	550 (96%)	22 (4%)	33	39
1	E	577/593 (97%)	552 (96%)	25 (4%)	29	33
1	F	573/593 (97%)	547 (96%)	26 (4%)	27	31
All	All	3442/3558 (97%)	3300 (96%)	142 (4%)	32	36

All (142) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	84	LEU
1	A	126[A]	GLU
1	A	126[B]	GLU
1	A	146	ASN
1	A	187	SER
1	A	313	GLN
1	A	329	THR
1	A	334	LEU
1	A	360	LYS
1	A	364	CYS
1	A	369	ASP
1	A	382	ASN
1	A	394	LEU
1	A	397[A]	SER
1	A	397[B]	SER
1	A	406	GLU
1	A	439	GLU
1	A	452	ASN
1	A	481[A]	LYS
1	A	481[B]	LYS
1	A	527	ASN
1	A	531	VAL
1	A	558	LEU
1	A	622	ILE
1	B	68	LYS
1	B	84	LEU
1	B	106	THR
1	B	109	LEU
1	B	201	LYS
1	B	213	ARG
1	B	217	LYS
1	B	238	GLU
1	B	265	LYS
1	B	313	GLN
1	B	329	THR
1	B	332	LEU
1	B	352	ARG
1	B	359	VAL
1	B	369	ASP
1	B	421	LEU
1	B	452	ASN
1	B	527	ASN

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Mol	Chain	Res	Type
1	B	576[A]	LYS
1	B	576[B]	LYS
1	B	633	LEU
1	C	20	ARG
1	C	102[A]	SER
1	C	102[B]	SER
1	C	125	GLU
1	C	146	ASN
1	C	157[A]	THR
1	C	157[B]	THR
1	C	202	LYS
1	C	213	ARG
1	C	313	GLN
1	C	329	THR
1	C	333	SER
1	C	334	LEU
1	C	360	LYS
1	C	364	CYS
1	C	382	ASN
1	C	394	LEU
1	C	425	LEU
1	C	452	ASN
1	C	527	ASN
1	C	531	VAL
1	C	558	LEU
1	C	641	LEU
1	C	670	ARG
1	D	20	ARG
1	D	48	LYS
1	D	77	ARG
1	D	109	LEU
1	D	118	VAL
1	D	125	GLU
1	D	136	GLU
1	D	143	ILE
1	D	248	GLU
1	D	313	GLN
1	D	334	LEU
1	D	352	ARG
1	D	397[A]	SER
1	D	397[B]	SER
1	D	421	LEU

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Mol	Chain	Res	Type
1	D	430	ASN
1	D	452	ASN
1	D	482	SER
1	D	527	ASN
1	D	558	LEU
1	D	633	LEU
1	D	642	MET
1	E	34	LYS
1	E	57	ARG
1	E	101	LEU
1	E	146	ASN
1	E	217	LYS
1	E	231	LYS
1	E	251	SER
1	E	254	MET
1	E	291	PRO
1	E	313	GLN
1	E	329	THR
1	E	360	LYS
1	E	364	CYS
1	E	382	ASN
1	E	394	LEU
1	E	452	ASN
1	E	517	SER
1	E	527	ASN
1	E	558	LEU
1	E	567[A]	SER
1	E	567[B]	SER
1	E	642	MET
1	E	644[A]	ARG
1	E	644[B]	ARG
1	E	672	VAL
1	F	20	ARG
1	F	48	LYS
1	F	84	LEU
1	F	109	LEU
1	F	122[A]	CYS
1	F	122[B]	CYS
1	F	126	GLU
1	F	148	MET
1	F	202	LYS
1	F	213	ARG

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Mol	Chain	Res	Type
1	F	226	LYS
1	F	253	LYS
1	F	288	ASN
1	F	313	GLN
1	F	329	THR
1	F	338	CYS
1	F	357	ILE
1	F	359	VAL
1	F	369	ASP
1	F	452	ASN
1	F	527	ASN
1	F	554	LYS
1	F	576[A]	LYS
1	F	576[B]	LYS
1	F	628	PRO
1	F	633	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (53) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	HIS
1	A	66	GLN
1	A	70	GLN
1	A	146	ASN
1	A	313	GLN
1	A	361	ASN
1	A	452	ASN
1	A	527	ASN
1	B	66	GLN
1	B	218	HIS
1	B	288	ASN
1	B	313	GLN
1	B	361	ASN
1	B	366	HIS
1	B	450	ASN
1	B	452	ASN
1	B	527	ASN
1	C	23	HIS
1	C	70	GLN
1	C	130	ASN
1	C	146	ASN
1	C	218	HIS

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Mol	Chain	Res	Type
1	C	263	ASN
1	C	313	GLN
1	C	361	ASN
1	C	452	ASN
1	C	527	ASN
1	D	218	HIS
1	D	288	ASN
1	D	313	GLN
1	D	361	ASN
1	D	366	HIS
1	D	450	ASN
1	D	452	ASN
1	D	527	ASN
1	E	23	HIS
1	E	66	GLN
1	E	146	ASN
1	E	171	GLN
1	E	263	ASN
1	E	286	HIS
1	E	313	GLN
1	E	361	ASN
1	E	452	ASN
1	E	527	ASN
1	F	70	GLN
1	F	218	HIS
1	F	286	HIS
1	F	288	ASN
1	F	313	GLN
1	F	450	ASN
1	F	452	ASN
1	F	527	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)

6 non-standard protein/DNA/RNA residues 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	$\#\|Z\| > 2$
1	TYQ	A	405	1	13,14,15	3.18	2 (15%)	15,19,21	2.16	3 (20%)
1	TYQ	F	405	1	13,14,15	3.41	2 (15%)	15,19,21	2.31	4 (26%)
1	TYQ	B	405	1	13,14,15	2.98	3 (23%)	15,19,21	3.47	10 (66%)
1	TYQ	D	405	1	13,14,15	2.67	2 (15%)	15,19,21	2.09	6 (40%)
1	TYQ	C	405	1	13,14,15	3.08	2 (15%)	15,19,21	2.40	5 (33%)
1	TYQ	E	405	1	13,14,15	2.32	3 (23%)	15,19,21	1.88	3 (20%)

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
1	TYQ	A	405	1	-	1/5/6/8	0/1/1/1
1	TYQ	F	405	1	-	2/5/6/8	0/1/1/1
1	TYQ	B	405	1	-	2/5/6/8	0/1/1/1
1	TYQ	D	405	1	-	2/5/6/8	0/1/1/1
1	TYQ	C	405	1	-	1/5/6/8	0/1/1/1
1	TYQ	E	405	1	-	1/5/6/8	0/1/1/1

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	405	TYQ	CE2-CZ	10.72	1.54	1.40
1	C	405	TYQ	CE2-CZ	8.54	1.51	1.40
1	A	405	TYQ	CE2-CZ	8.37	1.51	1.40
1	B	405	TYQ	CE2-CZ	7.12	1.49	1.40
1	A	405	TYQ	CD1-CG	7.02	1.50	1.40
1	E	405	TYQ	CE2-CZ	6.93	1.49	1.40
1	D	405	TYQ	CE2-CZ	6.82	1.49	1.40
1	C	405	TYQ	CD1-CG	6.48	1.49	1.40
1	B	405	TYQ	CD1-CG	6.37	1.49	1.40
1	D	405	TYQ	CD1-CG	6.03	1.48	1.40
1	F	405	TYQ	CD1-CG	5.69	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	405	TYQ	CE1-CZ	3.85	1.44	1.38
1	E	405	TYQ	CD1-CG	3.18	1.44	1.40
1	E	405	TYQ	CE1-CZ	2.17	1.42	1.38

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	405	TYQ	CB-CA-C	-7.47	97.47	111.47
1	C	405	TYQ	CB-CA-C	-7.04	98.27	111.47
1	A	405	TYQ	CB-CA-C	-6.54	99.20	111.47
1	B	405	TYQ	CB-CG-CD1	-6.17	114.49	120.95
1	B	405	TYQ	CD2-CG-CD1	5.22	124.45	118.17
1	F	405	TYQ	CB-CA-C	-5.08	101.94	111.47
1	D	405	TYQ	CB-CA-C	-5.04	102.02	111.47
1	E	405	TYQ	CB-CA-C	-4.88	102.32	111.47
1	F	405	TYQ	OH-CZ-CE2	4.55	123.86	116.25
1	F	405	TYQ	CZ-CE2-N5	3.93	125.02	118.77
1	C	405	TYQ	CG-CB-CA	-3.33	109.39	114.53
1	B	405	TYQ	CE1-CZ-CE2	3.22	122.51	119.44
1	B	405	TYQ	CE1-CD1-CG	-3.15	116.97	120.70
1	C	405	TYQ	CD2-CG-CD1	3.09	121.88	118.17
1	B	405	TYQ	CG-CB-CA	-3.08	109.76	114.53
1	C	405	TYQ	CB-CG-CD1	-2.98	117.83	120.95
1	A	405	TYQ	CE1-CZ-CE2	2.93	122.23	119.44
1	D	405	TYQ	CE1-CD1-CG	-2.92	117.25	120.70
1	B	405	TYQ	OH-CZ-CE2	-2.83	111.52	116.25
1	D	405	TYQ	CZ-CE1-CD1	2.73	122.85	120.14
1	E	405	TYQ	CG-CB-CA	2.70	118.70	114.53
1	A	405	TYQ	CD2-CG-CD1	2.67	121.37	118.17
1	D	405	TYQ	OH-CZ-CE2	2.65	120.69	116.25
1	F	405	TYQ	CD2-CG-CD1	2.65	121.35	118.17
1	B	405	TYQ	CD2-CE2-N5	2.53	126.09	119.43
1	D	405	TYQ	CD2-CG-CD1	2.44	121.10	118.17
1	B	405	TYQ	OH-CZ-CE1	2.43	125.96	119.46
1	E	405	TYQ	OH-CZ-CE1	2.26	125.51	119.46
1	B	405	TYQ	OZ-CD1-CE1	2.19	125.33	119.46
1	D	405	TYQ	CZ-CE2-N5	2.18	122.25	118.77
1	C	405	TYQ	OH-CZ-CE2	2.03	119.65	116.25

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B	405	TYQ	O-C-CA-CB
1	D	405	TYQ	N-CA-CB-CG
1	E	405	TYQ	N-CA-CB-CG
1	F	405	TYQ	O-C-CA-CB
1	F	405	TYQ	N-CA-CB-CG
1	A	405	TYQ	N-CA-CB-CG
1	B	405	TYQ	N-CA-CB-CG
1	C	405	TYQ	N-CA-CB-CG
1	D	405	TYQ	C-CA-CB-CG

There are no ring outliers.

6 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	405	TYQ	3	0
1	F	405	TYQ	3	0
1	B	405	TYQ	2	0
1	D	405	TYQ	2	0
1	C	405	TYQ	3	0
1	E	405	TYQ	2	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 46 ligands modelled in this entry, 6 are monoatomic - leaving 40 for Mogul analysis.

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	$\#\|Z\| > 2$
2	GOL	C	702	-	5,5,5	0.33	0	5,5,5	0.33	0
2	GOL	C	704	-	5,5,5	0.55	0	5,5,5	0.69	0
4	PEO	E	705	-	1,1,1	0.07	0	-		
2	GOL	F	703	-	5,5,5	0.64	0	5,5,5	0.69	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	GOL	A	701	-	5,5,5	0.45	0	5,5,5	0.42	0
5	ABN	E	707	-	8,8,8	0.55	0	9,9,9	0.47	0
2	GOL	A	705	-	5,5,5	0.44	0	5,5,5	0.42	0
2	GOL	D	704	-	5,5,5	0.34	0	5,5,5	0.49	0
2	GOL	B	705	-	5,5,5	0.53	0	5,5,5	1.08	0
2	GOL	A	704	-	5,5,5	0.46	0	5,5,5	0.25	0
5	ABN	D	706	-	8,8,8	1.16	0	9,9,9	1.07	1 (11%)
4	PEO	F	707	-	1,1,1	0.13	0	-		
2	GOL	C	705	-	5,5,5	0.62	0	5,5,5	0.66	0
2	GOL	B	707	-	5,5,5	0.37	0	5,5,5	1.00	0
2	GOL	C	707	-	5,5,5	0.52	0	5,5,5	1.50	1 (20%)
2	GOL	E	703	-	5,5,5	0.25	0	5,5,5	1.05	0
5	ABN	C	708	-	8,8,8	1.12	0	9,9,9	0.55	0
5	ABN	F	708	-	8,8,8	0.60	0	9,9,9	0.26	0
2	GOL	E	704	-	5,5,5	0.29	0	5,5,5	0.80	0
2	GOL	E	706	-	5,5,5	0.43	0	5,5,5	0.95	0
2	GOL	C	706	-	5,5,5	0.47	0	5,5,5	0.85	0
4	PEO	A	707	-	1,1,1	0.57	0	-		
2	GOL	B	704	-	5,5,5	0.55	0	5,5,5	1.07	0
2	GOL	E	702	-	5,5,5	0.44	0	5,5,5	0.66	0
4	PEO	B	708	3	1,1,1	0.21	0	-		
2	GOL	B	706	-	5,5,5	0.36	0	5,5,5	0.92	0
2	GOL	A	706	-	5,5,5	0.41	0	5,5,5	0.47	0
5	ABN	B	709	-	8,8,8	1.24	1 (12%)	9,9,9	1.70	2 (22%)
2	GOL	D	703	-	5,5,5	0.81	0	5,5,5	0.56	0
2	GOL	D	705	-	5,5,5	0.51	0	5,5,5	0.57	0
2	GOL	B	701	-	5,5,5	0.57	0	5,5,5	0.94	0
2	GOL	A	703	-	5,5,5	0.41	0	5,5,5	0.86	0
2	GOL	F	705	-	5,5,5	0.36	0	5,5,5	1.12	0
2	GOL	B	703	-	5,5,5	0.81	0	5,5,5	0.70	0
5	ABN	A	708	-	8,8,8	0.67	0	9,9,9	0.79	0
2	GOL	D	702	-	5,5,5	0.43	0	5,5,5	0.66	0
2	GOL	F	702	-	5,5,5	0.61	0	5,5,5	0.95	0
2	GOL	F	704	-	5,5,5	0.34	0	5,5,5	0.61	0
2	GOL	F	706	-	5,5,5	0.40	0	5,5,5	0.86	0
2	GOL	C	703	-	5,5,5	0.36	0	5,5,5	0.96	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
2	GOL	C	702	-	-	4/4/4/4	-
2	GOL	C	704	-	-	2/4/4/4	-
2	GOL	F	703	-	-	4/4/4/4	-
2	GOL	A	701	-	-	0/4/4/4	-
5	ABN	E	707	-	-	0/2/2/2	0/1/1/1
2	GOL	A	705	-	-	2/4/4/4	-
2	GOL	D	704	-	-	2/4/4/4	-
2	GOL	B	705	-	-	1/4/4/4	-
2	GOL	A	704	-	-	1/4/4/4	-
5	ABN	D	706	-	-	1/2/2/2	0/1/1/1
2	GOL	C	705	-	-	2/4/4/4	-
2	GOL	B	707	-	-	4/4/4/4	-
2	GOL	C	707	-	-	0/4/4/4	-
2	GOL	E	703	-	-	4/4/4/4	-
5	ABN	C	708	-	-	0/2/2/2	0/1/1/1
5	ABN	F	708	-	-	0/2/2/2	0/1/1/1
2	GOL	E	704	-	-	2/4/4/4	-
2	GOL	E	706	-	-	4/4/4/4	-
2	GOL	C	706	-	-	2/4/4/4	-
2	GOL	B	704	-	-	3/4/4/4	-
2	GOL	E	702	-	-	2/4/4/4	-
2	GOL	B	706	-	-	2/4/4/4	-
2	GOL	A	706	-	-	4/4/4/4	-
5	ABN	B	709	-	-	0/2/2/2	0/1/1/1
2	GOL	D	703	-	-	4/4/4/4	-
2	GOL	D	705	-	-	3/4/4/4	-
2	GOL	B	701	-	-	2/4/4/4	-
2	GOL	A	703	-	-	1/4/4/4	-
2	GOL	F	705	-	-	3/4/4/4	-
2	GOL	B	703	-	-	2/4/4/4	-
5	ABN	A	708	-	-	0/2/2/2	0/1/1/1
2	GOL	D	702	-	-	2/4/4/4	-
2	GOL	F	702	-	-	4/4/4/4	-
2	GOL	F	704	-	-	2/4/4/4	-
2	GOL	F	706	-	-	3/4/4/4	-
2	GOL	C	703	-	-	2/4/4/4	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	709	ABN	C3-C2	2.28	1.43	1.38

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	709	ABN	C3-C2-C1	3.01	125.25	120.63
5	B	709	ABN	C4-C5-C6	2.67	124.27	120.19
5	D	706	ABN	C4-C5-C6	-2.31	116.67	120.19
2	C	707	GOL	C3-C2-C1	-2.01	103.88	111.70

There are no chirality outliers.

All (74) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	705	GOL	O1-C1-C2-C3
2	A	706	GOL	C1-C2-C3-O3
2	B	701	GOL	O1-C1-C2-C3
2	B	704	GOL	O1-C1-C2-C3
2	B	704	GOL	O2-C2-C3-O3
2	B	707	GOL	C1-C2-C3-O3
2	C	702	GOL	O1-C1-C2-C3
2	C	704	GOL	O1-C1-C2-O2
2	C	704	GOL	O1-C1-C2-C3
2	C	705	GOL	O1-C1-C2-C3
2	D	703	GOL	O1-C1-C2-O2
2	D	703	GOL	O1-C1-C2-C3
2	D	703	GOL	C1-C2-C3-O3
2	D	703	GOL	O2-C2-C3-O3
2	D	704	GOL	O1-C1-C2-C3
2	E	702	GOL	O1-C1-C2-O2
2	E	702	GOL	O1-C1-C2-C3
2	E	706	GOL	O1-C1-C2-C3
2	F	703	GOL	O1-C1-C2-O2
2	F	703	GOL	O1-C1-C2-C3
2	F	703	GOL	C1-C2-C3-O3
2	F	703	GOL	O2-C2-C3-O3
2	F	704	GOL	C1-C2-C3-O3
2	F	705	GOL	C1-C2-C3-O3
2	F	705	GOL	O2-C2-C3-O3
2	A	705	GOL	O1-C1-C2-O2
2	A	706	GOL	O2-C2-C3-O3
2	F	702	GOL	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
2	A	703	GOL	C1-C2-C3-O3
2	A	706	GOL	O1-C1-C2-C3
2	B	703	GOL	C1-C2-C3-O3
2	B	704	GOL	C1-C2-C3-O3
2	B	706	GOL	O1-C1-C2-C3
2	B	707	GOL	O1-C1-C2-C3
2	C	702	GOL	C1-C2-C3-O3
2	C	703	GOL	C1-C2-C3-O3
2	C	706	GOL	C1-C2-C3-O3
2	D	702	GOL	O1-C1-C2-C3
2	D	705	GOL	C1-C2-C3-O3
2	E	703	GOL	O1-C1-C2-C3
2	E	703	GOL	C1-C2-C3-O3
2	E	704	GOL	C1-C2-C3-O3
2	E	706	GOL	C1-C2-C3-O3
2	F	702	GOL	O1-C1-C2-C3
2	F	702	GOL	C1-C2-C3-O3
2	F	706	GOL	O1-C1-C2-C3
2	F	706	GOL	C1-C2-C3-O3
2	B	707	GOL	O1-C1-C2-O2
2	C	702	GOL	O1-C1-C2-O2
2	C	702	GOL	O2-C2-C3-O3
2	C	705	GOL	O1-C1-C2-O2
2	C	706	GOL	O2-C2-C3-O3
2	D	704	GOL	O1-C1-C2-O2
2	E	706	GOL	O1-C1-C2-O2
2	F	702	GOL	O1-C1-C2-O2
2	F	704	GOL	O2-C2-C3-O3
2	F	706	GOL	O2-C2-C3-O3
2	B	707	GOL	O2-C2-C3-O3
2	E	703	GOL	O1-C1-C2-O2
2	E	703	GOL	O2-C2-C3-O3
2	B	701	GOL	O1-C1-C2-O2
2	C	703	GOL	O2-C2-C3-O3
2	D	702	GOL	O1-C1-C2-O2
2	E	704	GOL	O2-C2-C3-O3
2	E	706	GOL	O2-C2-C3-O3
2	B	703	GOL	O2-C2-C3-O3
2	B	706	GOL	O1-C1-C2-O2
2	B	705	GOL	C1-C2-C3-O3
2	D	705	GOL	O2-C2-C3-O3
2	F	705	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
2	A	706	GOL	O1-C1-C2-O2
5	D	706	ABN	N-C-C1-C2
2	A	704	GOL	O1-C1-C2-O2
2	D	705	GOL	O1-C1-C2-C3

There are no ring outliers.

24 monomers are involved in 55 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	702	GOL	2	0
5	E	707	ABN	2	0
2	D	704	GOL	1	0
5	D	706	ABN	3	0
4	F	707	PEO	1	0
2	B	707	GOL	1	0
2	C	707	GOL	1	0
5	C	708	ABN	5	0
5	F	708	ABN	3	0
2	E	704	GOL	3	0
2	E	706	GOL	3	0
4	A	707	PEO	1	0
2	B	704	GOL	1	0
2	B	706	GOL	2	0
5	B	709	ABN	2	0
2	D	705	GOL	1	0
2	A	703	GOL	6	0
2	F	705	GOL	1	0
2	B	703	GOL	1	0
5	A	708	ABN	2	0
2	D	702	GOL	7	0
2	F	702	GOL	4	0
2	F	704	GOL	1	0
2	C	703	GOL	1	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	653/692 (94%)	0.06	23 (3%)	44	46	15, 31, 53, 86	0
1	B	654/692 (94%)	-0.08	8 (1%)	79	81	15, 27, 45, 67	0
1	C	654/692 (94%)	0.02	27 (4%)	37	40	20, 32, 54, 84	0
1	D	654/692 (94%)	0.31	59 (9%)	9	10	22, 37, 60, 89	0
1	E	653/692 (94%)	0.18	26 (3%)	38	40	18, 33, 54, 83	0
1	F	654/692 (94%)	0.06	19 (2%)	51	55	15, 31, 54, 76	0
All	All	3922/4152 (94%)	0.09	162 (4%)	37	40	15, 32, 55, 89	0

All (162) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	18	PRO	6.9
1	A	19	ALA	6.6
1	D	18	PRO	6.6
1	E	672	VAL	6.3
1	F	672	VAL	5.9
1	E	334	LEU	5.8
1	F	334	LEU	5.8
1	E	20	ARG	5.4
1	E	46	GLY	5.2
1	D	672	VAL	5.0
1	C	334	LEU	4.8
1	D	46	GLY	4.7
1	C	247	PRO	4.6
1	B	17	ALA	4.5
1	D	423	ILE	4.5
1	E	21	PRO	4.5
1	B	334	LEU	4.5
1	D	21	PRO	4.3
1	E	671	ALA	4.2

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Mol	Chain	Res	Type	RSRZ
1	D	19	ALA	4.2
1	F	19	ALA	4.0
1	D	122[A]	CYS	3.8
1	D	639	ILE	3.7
1	D	135	ILE	3.7
1	F	20	ARG	3.6
1	D	142	GLY	3.5
1	C	670	ARG	3.5
1	D	671	ALA	3.5
1	D	409	LEU	3.5
1	E	423	ILE	3.5
1	E	19	ALA	3.5
1	A	22	ALA	3.4
1	D	22	ALA	3.4
1	A	101	LEU	3.3
1	D	638	PRO	3.3
1	D	20	ARG	3.3
1	E	101	LEU	3.2
1	D	421	LEU	3.2
1	B	437	ASP	3.2
1	C	237	PRO	3.2
1	E	44	PHE	3.1
1	A	421	LEU	3.1
1	D	146	ASN	3.1
1	F	437	ASP	3.1
1	A	407	TYR	3.1
1	A	423	ILE	3.1
1	F	335	GLY	3.0
1	A	671	ALA	3.0
1	E	45	ALA	3.0
1	C	672	VAL	3.0
1	A	21	PRO	3.0
1	D	334	LEU	2.9
1	E	43	TYR	2.9
1	C	638	PRO	2.9
1	C	544	VAL	2.9
1	D	640	THR	2.9
1	D	622	ILE	2.9
1	C	671	ALA	2.9
1	D	250	VAL	2.8
1	A	334	LEU	2.8
1	D	247	PRO	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	99	ALA	2.8
1	B	22	ALA	2.8
1	D	353	ALA	2.8
1	B	340	GLY	2.8
1	D	460	PHE	2.8
1	E	130	ASN	2.8
1	E	48	LYS	2.8
1	D	147	GLU	2.8
1	A	333	SER	2.7
1	C	242	ILE	2.7
1	D	335	GLY	2.7
1	F	21	PRO	2.7
1	E	100	SER	2.7
1	D	121	LEU	2.7
1	F	639	ILE	2.7
1	A	46	GLY	2.7
1	E	249	GLY	2.7
1	A	39	THR	2.7
1	D	621	GLY	2.7
1	D	644[A]	ARG	2.7
1	F	48	LYS	2.7
1	D	42	SER	2.7
1	D	132	PRO	2.7
1	C	423	ILE	2.7
1	E	320	ILE	2.7
1	C	641	LEU	2.6
1	A	45	ALA	2.6
1	D	544	VAL	2.6
1	C	241	PRO	2.5
1	A	425	LEU	2.5
1	E	408	CYS	2.5
1	C	139	VAL	2.5
1	F	102	SER	2.5
1	E	333	SER	2.5
1	C	437[A]	ASP	2.5
1	E	336[A]	CYS	2.5
1	E	421	LEU	2.5
1	C	634[A]	MET	2.4
1	C	336	CYS	2.4
1	A	42[A]	SER	2.4
1	F	671	ALA	2.4
1	C	640	THR	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	245	THR	2.4
1	D	38	ASN	2.4
1	D	459	LEU	2.4
1	D	336	CYS	2.4
1	D	408	CYS	2.4
1	C	245	THR	2.4
1	D	45	ALA	2.3
1	A	249	GLY	2.3
1	E	298	LEU	2.3
1	E	634[A]	MET	2.3
1	C	233	GLY	2.3
1	D	143	ILE	2.3
1	C	22	ALA	2.3
1	D	126	GLU	2.3
1	A	641	LEU	2.3
1	C	643	LEU	2.3
1	D	44	PHE	2.3
1	C	668	ALA	2.3
1	C	543	LEU	2.3
1	B	211[A]	ARG	2.3
1	B	622	ILE	2.3
1	A	20	ARG	2.2
1	D	287	GLY	2.2
1	F	18	PRO	2.2
1	E	22	ALA	2.2
1	C	621	GLY	2.2
1	D	130	ASN	2.2
1	C	658	GLN	2.2
1	D	102	SER	2.2
1	F	46	GLY	2.2
1	A	639	ILE	2.2
1	F	135	ILE	2.2
1	D	425	LEU	2.2
1	B	247	PRO	2.2
1	A	670	ARG	2.1
1	D	127	VAL	2.1
1	F	336	CYS	2.1
1	D	244	VAL	2.1
1	D	426	THR	2.1
1	C	425	LEU	2.1
1	D	301	MET	2.1
1	F	139	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	248	GLU	2.1
1	D	35	ALA	2.1
1	D	40	VAL	2.1
1	E	638	PRO	2.1
1	D	48	LYS	2.1
1	D	240	PRO	2.1
1	D	243	ASN	2.0
1	E	247	PRO	2.0
1	D	67	TRP	2.0
1	A	48	LYS	2.0
1	F	640	THR	2.0
1	F	234	ALA	2.0
1	F	670	ARG	2.0
1	D	229	ILE	2.0
1	D	298	LEU	2.0
1	D	340	GLY	2.0
1	D	255	THR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (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
1	TYQ	D	405	14/15	0.91	0.21	38,42,46,47	0
1	TYQ	B	405	14/15	0.93	0.16	22,26,33,36	0
1	TYQ	C	405	14/15	0.93	0.20	28,35,42,43	0
1	TYQ	A	405	14/15	0.93	0.20	23,31,35,35	0
1	TYQ	E	405	14/15	0.94	0.20	23,29,40,42	0
1	TYQ	F	405	14/15	0.94	0.16	28,36,44,46	0

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
2	GOL	D	705	6/6	0.70	0.29	70,72,73,74	0
2	GOL	E	703	6/6	0.79	0.24	64,65,66,67	0
2	GOL	A	704	6/6	0.82	0.21	59,64,67,67	0
2	GOL	C	707	6/6	0.82	0.18	45,55,56,60	0
2	GOL	B	705	6/6	0.83	0.29	62,64,67,70	0
2	GOL	B	704	6/6	0.83	0.25	41,49,51,55	0
2	GOL	F	706	6/6	0.83	0.30	57,57,60,60	0
2	GOL	F	705	6/6	0.84	0.26	61,65,66,68	0
2	GOL	E	704	6/6	0.85	0.23	66,69,70,71	0
2	GOL	D	704	6/6	0.86	0.24	52,58,61,63	0
2	GOL	F	704	6/6	0.86	0.29	46,52,53,56	0
2	GOL	B	707	6/6	0.87	0.16	50,52,53,55	0
2	GOL	C	704	6/6	0.87	0.26	52,56,56,60	0
5	ABN	B	709	8/8	0.87	0.23	40,42,44,44	0
2	GOL	A	706	6/6	0.88	0.34	56,61,66,69	0
2	GOL	D	703	6/6	0.89	0.18	51,54,56,57	0
2	GOL	C	706	6/6	0.89	0.24	62,64,67,68	0
2	GOL	C	705	6/6	0.89	0.13	62,64,65,66	0
2	GOL	A	705	6/6	0.90	0.28	50,52,53,54	0
2	GOL	E	706	6/6	0.90	0.18	52,55,56,57	0
2	GOL	C	702	6/6	0.90	0.13	49,57,59,61	0
2	GOL	C	703	6/6	0.91	0.30	46,49,50,53	0
2	GOL	D	702	6/6	0.91	0.17	57,60,61,62	0
2	GOL	B	703	6/6	0.91	0.20	46,49,50,50	0
5	ABN	C	708	8/8	0.91	0.19	38,39,41,42	0
5	ABN	D	706	8/8	0.91	0.20	36,37,37,38	0
2	GOL	F	702	6/6	0.92	0.22	44,51,52,55	0
2	GOL	F	703	6/6	0.92	0.22	62,65,65,66	0
2	GOL	E	702	6/6	0.92	0.30	55,58,60,60	0
2	GOL	A	703	6/6	0.92	0.17	51,56,57,60	0
5	ABN	A	708	8/8	0.94	0.19	31,32,34,37	0
2	GOL	B	701	6/6	0.94	0.23	27,33,35,36	0
2	GOL	B	706	6/6	0.95	0.21	50,52,54,57	0
5	ABN	F	708	8/8	0.95	0.17	38,41,42,42	0
4	PEO	F	707	2/2	0.96	0.22	28,28,28,36	0
5	ABN	E	707	8/8	0.96	0.19	32,33,34,35	0
4	PEO	B	708	2/2	0.96	0.20	24,24,24,26	0
4	PEO	E	705	2/2	0.97	0.34	30,30,30,35	0
4	PEO	A	707	2/2	0.98	0.25	26,26,26,31	0
2	GOL	A	701	6/6	0.98	0.13	32,34,37,42	0
3	CU	E	701	1/1	0.99	0.14	28,28,28,28	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	CU	F	701	1/1	0.99	0.12	31,31,31,31	0
3	CU	C	701	1/1	0.99	0.12	33,33,33,33	0
3	CU	D	701	1/1	0.99	0.13	36,36,36,36	0
3	CU	A	702	1/1	1.00	0.14	28,28,28,28	0
3	CU	B	702	1/1	1.00	0.12	26,26,26,26	0

6.5 Other polymers (i)

There are no such residues in this entry.