Full wwPDB X-ray Structure Validation Report (i)

Sep 17, 2023 – 10:10 AM EDT

PDB ID	:	4Y97
Title	:	Crystal Structure of human Pol alpha B-subunit in complex with C-terminal domain of catalytic subunit
Authors	:	Suwa, Y.; Gu, J.; Baranovskiy, A.G.; Babayeva, N.D.; Tahirov, T.H.
Deposited on	:	2015-02-17
Resolution	:	2.51 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 (1)) were used in the production of this report:

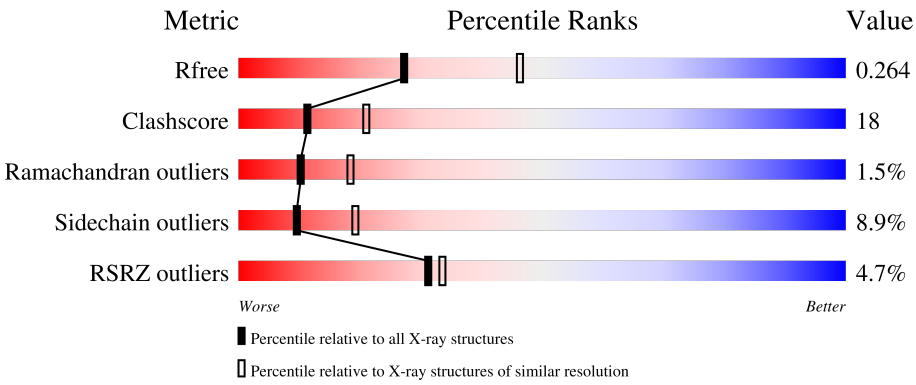
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 2.51 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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	598	2%, 50%, 21%, •, 26%
1	C	598	2%, 51%, 19%, •, •, 26%
1	E	598	%, 53%, 17%, •, 27%
1	G	598	2%, 47%, 21%, 5%, •, 27%
2	B	180	10%, 56%, 35%, 6%, •

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Mol	Chain	Length	Quality of chain
2	D	180	8% 66% 27% 6%
2	F	180	4% 61% 33%
2	H	180	20% 57% 38%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 19724 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 DNA polymerase alpha subunit B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	442	3439	2187	574	663	15	0	0	0
1	C	441	3435	2187	573	660	15	0	0	0
1	E	439	3422	2178	571	658	15	0	0	0
1	G	436	3400	2164	568	653	15	0	0	0

- Molecule 2 is a protein called DNA polymerase alpha catalytic subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	173	1426	902	240	269	15	0	0	0
2	D	178	1466	926	248	277	15	0	0	0
2	F	176	1451	919	244	273	15	0	0	0
2	H	179	1475	931	250	279	15	0	0	0

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
3	B	2	2	2	0	0
3	D	2	2	2	0	0
3	F	2	2	2	0	0
3	H	2	2	2	0	0

- Molecule 4 is water.

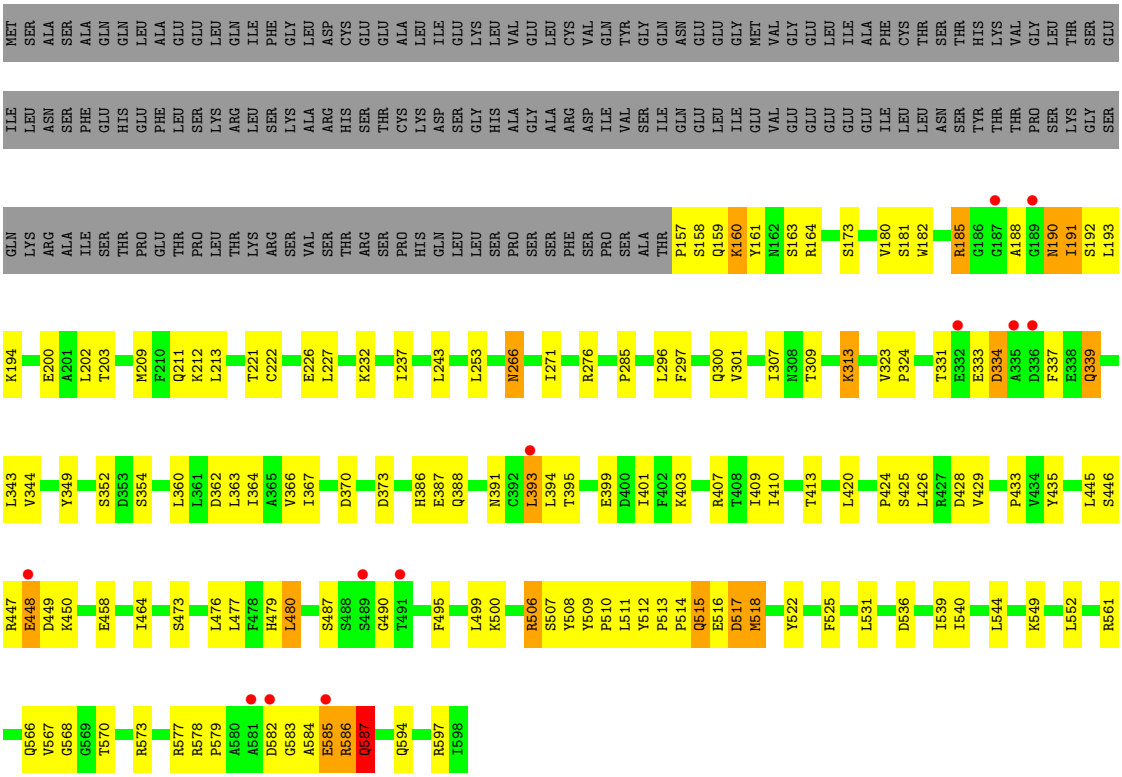
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	37	37	37	0	0
			Total	O		
4	B	8	8	8	0	0
			Total	O		
4	C	63	63	63	0	0
			Total	O		
4	D	24	24	24	0	0
			Total	O		
4	E	39	39	39	0	0
			Total	O		
4	F	14	14	14	0	0
			Total	O		
4	G	13	13	13	0	0
			Total	O		
4	H	4	4	4	0	0

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.

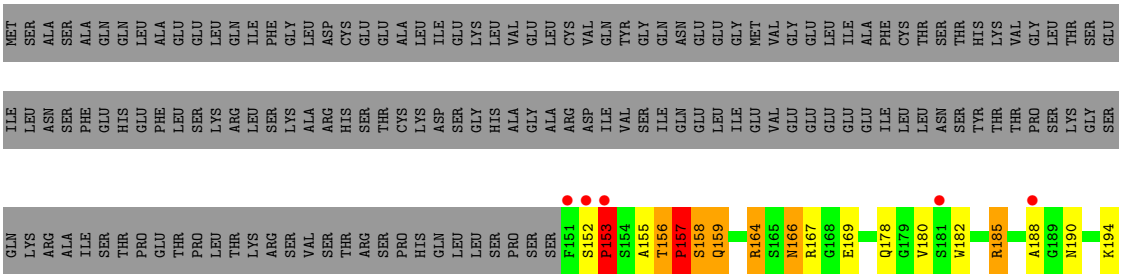
• Molecule 1: DNA polymerase alpha subunit B

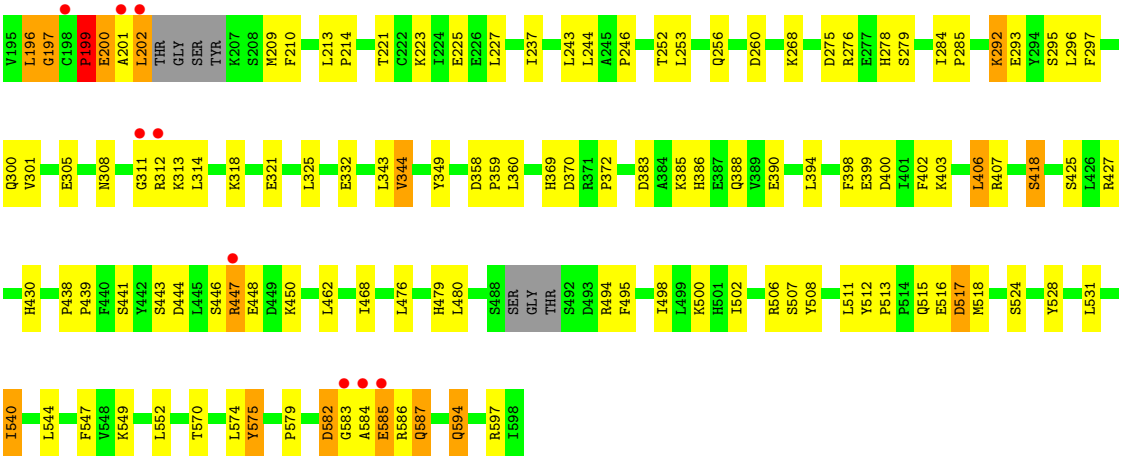
Chain A: 2% 50% 21% • 26%



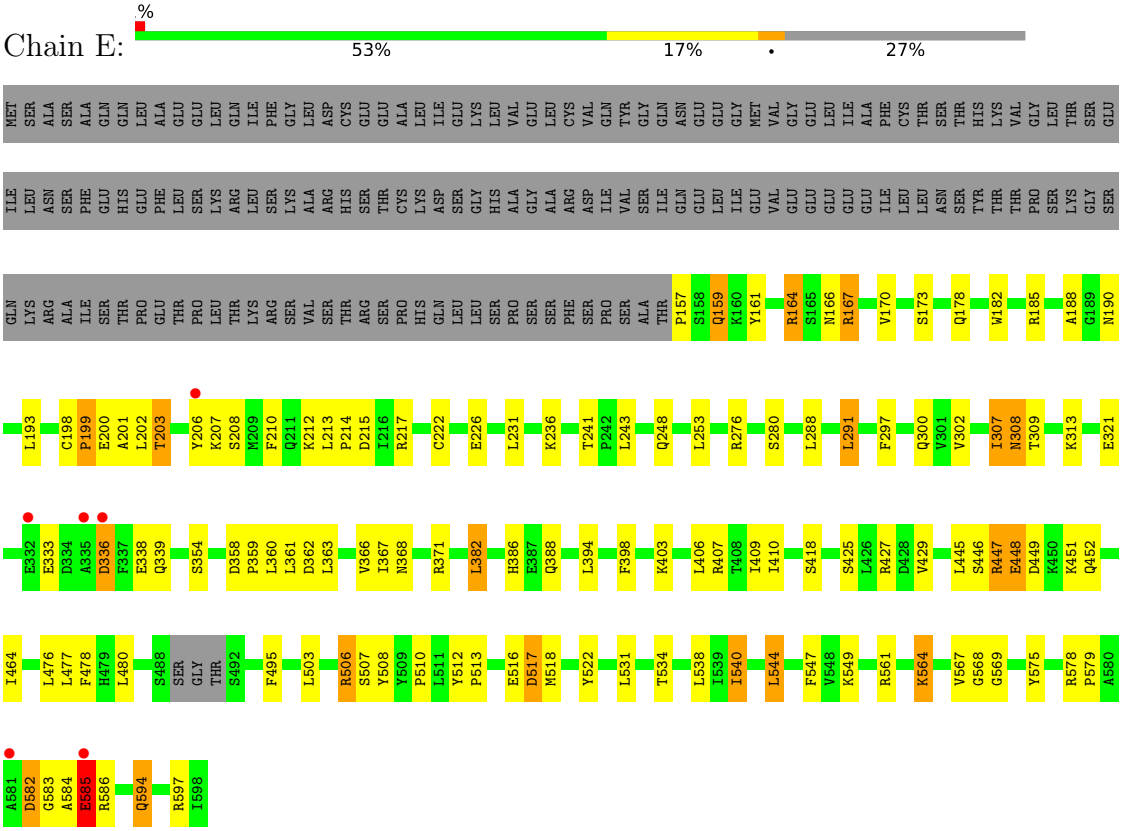
• Molecule 1: DNA polymerase alpha subunit B

Chain C: 2% 51% 19% • • 26%

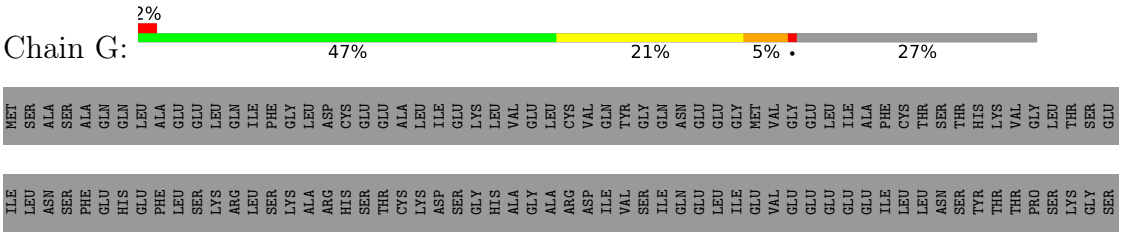


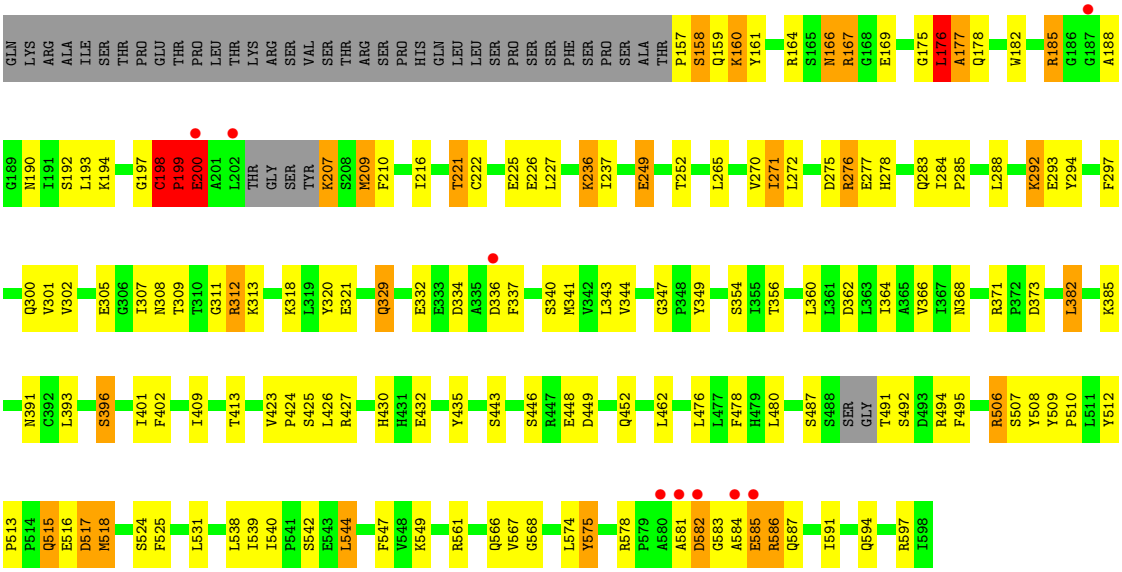


• Molecule 1: DNA polymerase alpha subunit B



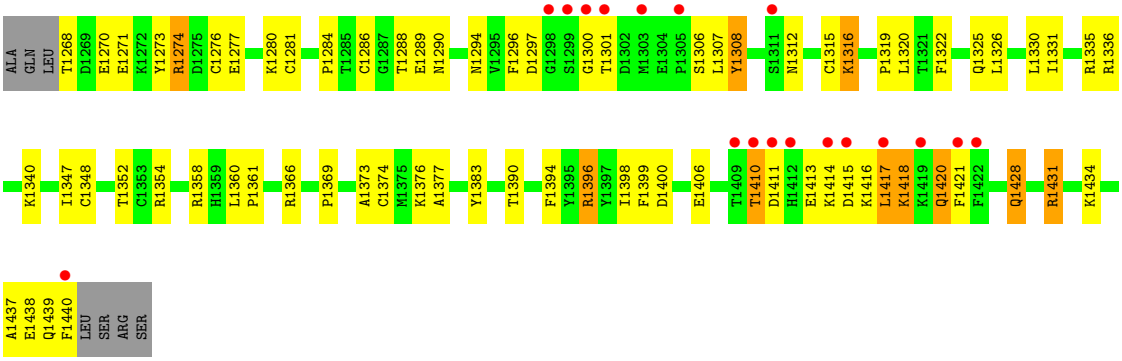
• Molecule 1: DNA polymerase alpha subunit B





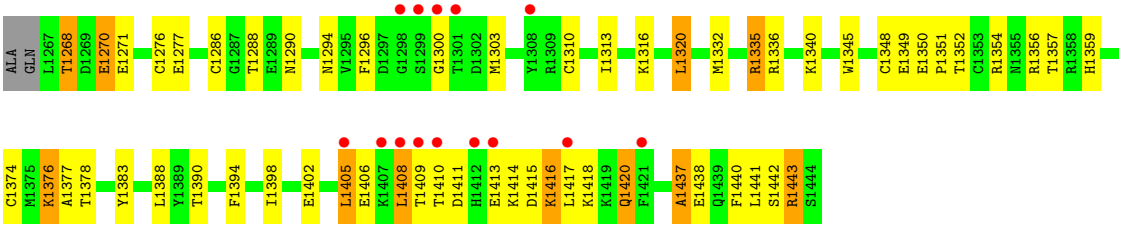
- Molecule 2: DNA polymerase alpha catalytic subunit

Chain B:



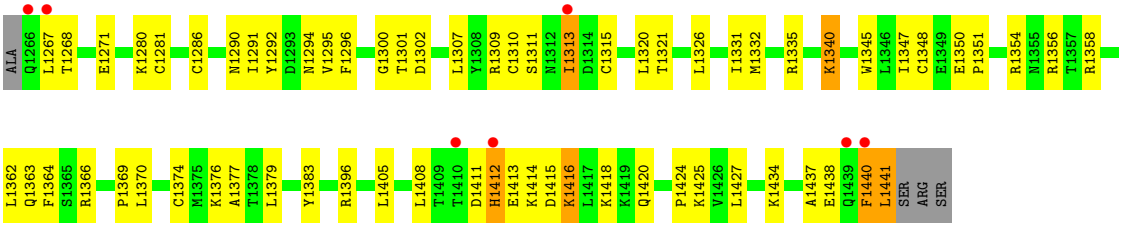
- Molecule 2: DNA polymerase alpha catalytic subunit

Chain D:



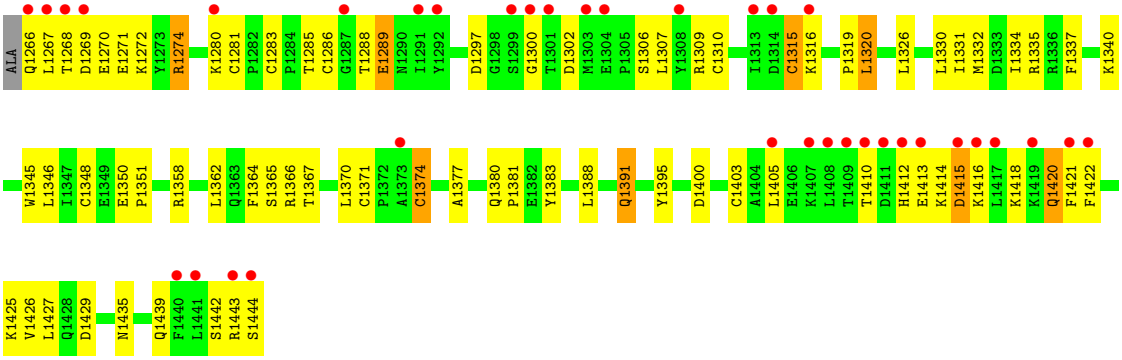
- Molecule 2: DNA polymerase alpha catalytic subunit

Chain F:



- Molecule 2: DNA polymerase alpha catalytic subunit

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	103.59Å 137.13Å 132.09Å 90.00° 100.97° 90.00°	Depositor
Resolution (Å)	47.68 – 2.51 47.68 – 2.51	Depositor EDS
% Data completeness (in resolution range)	94.2 (47.68-2.51) 94.3 (47.68-2.51)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.07 (at 2.51Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.218 , 0.257 0.228 , 0.264	Depositor DCC
R_{free} test set	5894 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	31.2	Xtriage
Anisotropy	0.639	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 53.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	19724	wwPDB-VP
Average B, all atoms (Å^2)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.36% 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: ZN

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	0.43	0/3517	0.74	1/4777 (0.0%)
1	C	0.49	0/3512	0.84	7/4769 (0.1%)
1	E	0.46	0/3499	0.77	3/4751 (0.1%)
1	G	0.39	0/3475	0.78	8/4717 (0.2%)
2	B	0.43	0/1459	0.69	2/1967 (0.1%)
2	D	0.44	0/1499	0.67	1/2019 (0.0%)
2	F	0.42	0/1484	0.71	1/2001 (0.0%)
2	H	0.40	0/1508	0.68	1/2031 (0.0%)
All	All	0.44	0/19953	0.76	24/27032 (0.1%)

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	E	0	1

There are no bond length outliers.

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	156	THR	C-N-CD	-20.28	75.98	120.60
1	G	198	CYS	N-CA-C	-10.39	82.94	111.00
1	C	156	THR	C-N-CA	9.90	163.59	122.00
1	G	198	CYS	C-N-CD	-9.72	99.21	120.60
1	G	197	GLY	N-CA-C	7.01	130.63	113.10
2	B	1439	GLN	N-CA-C	-6.96	92.21	111.00
1	C	390	GLU	CA-CB-CG	6.46	127.62	113.40
1	E	210	PHE	N-CA-C	-5.78	95.38	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	197	GLY	C-N-CA	5.66	135.84	121.70
2	F	1374	CYS	N-CA-C	-5.62	95.83	111.00
1	G	198	CYS	C-N-CA	5.59	145.50	122.00
2	B	1374	CYS	N-CA-C	-5.55	96.01	111.00
1	C	582	ASP	N-CA-C	5.54	125.95	111.00
2	H	1374	CYS	N-CA-C	-5.54	96.04	111.00
2	D	1374	CYS	N-CA-C	-5.39	96.43	111.00
1	G	200	GLU	N-CA-C	5.30	125.31	111.00
1	C	587	GLN	N-CA-C	-5.28	96.75	111.00
1	A	587	GLN	N-CA-C	-5.23	96.88	111.00
1	G	582	ASP	N-CA-C	5.13	124.86	111.00
1	E	582	ASP	N-CA-C	5.11	124.80	111.00
1	C	153	PRO	N-CA-C	5.09	125.33	112.10
1	C	157	PRO	CA-N-CD	-5.08	104.39	111.50
1	E	178	GLN	N-CA-C	-5.06	97.33	111.00
1	G	587	GLN	N-CA-C	-5.03	97.43	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	522	TYR	Sidechain

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	3439	0	3414	134	0
1	C	3435	0	3410	132	0
1	E	3422	0	3398	78	0
1	G	3400	0	3380	144	0
2	B	1426	0	1389	53	0
2	D	1466	0	1434	50	0
2	F	1451	0	1419	63	0
2	H	1475	0	1442	72	0
3	B	2	0	0	0	0
3	D	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	F	2	0	0	0	0
3	H	2	0	0	0	0
4	A	37	0	0	3	0
4	B	8	0	0	0	0
4	C	63	0	0	3	0
4	D	24	0	0	2	0
4	E	39	0	0	4	0
4	F	14	0	0	2	0
4	G	13	0	0	2	0
4	H	4	0	0	0	0
All	All	19724	0	19286	691	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 18.

All (691) 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:161:TYR:O	1:E:164:ARG:HD2	1.42	1.16
1:G:209:MET:HB2	2:H:1443:ARG:HB3	1.30	1.11
1:C:185:ARG:HH11	1:C:185:ARG:HB3	1.06	1.08
1:C:166:ASN:H	1:C:166:ASN:ND2	1.46	1.08
1:G:169:GLU:HB3	1:G:597:ARG:HD2	1.40	1.03
1:C:166:ASN:HD22	1:C:166:ASN:N	1.54	1.03
1:E:164:ARG:HG3	1:E:164:ARG:HH11	1.23	1.01
2:H:1307:LEU:O	2:H:1319:PRO:HG2	1.62	1.00
1:C:152:SER:HB3	1:C:153:PRO:HD2	1.43	0.98
1:A:157:PRO:O	1:A:159:GLN:N	1.97	0.96
1:G:198:CYS:N	1:G:199:PRO:HD3	1.79	0.95
2:F:1267:LEU:HD22	2:F:1271:GLU:HG3	1.48	0.95
2:H:1412:HIS:O	2:H:1416:LYS:HG3	1.67	0.94
2:F:1313:ILE:HD13	2:F:1313:ILE:H	1.34	0.92
1:C:246:PRO:HG3	1:C:311:GLY:HA3	1.49	0.91
1:A:160:LYS:HE3	1:A:160:LYS:H	1.32	0.91
2:D:1376:LYS:HE2	2:D:1376:LYS:HA	1.52	0.91
2:B:1288:THR:HG21	2:B:1312:ASN:HB2	1.50	0.90
1:C:495:PHE:HB2	1:C:549:LYS:HE3	1.54	0.90
2:F:1268:THR:HG22	2:F:1271:GLU:HG2	1.54	0.89
1:G:198:CYS:N	1:G:199:PRO:CD	2.28	0.89
2:D:1313:ILE:HD12	2:D:1313:ILE:H	1.35	0.88
1:G:209:MET:HB2	2:H:1443:ARG:CB	2.04	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:160:LYS:H	1:A:160:LYS:CE	1.86	0.87
1:A:506:ARG:HG2	1:A:506:ARG:HH11	1.40	0.87
1:C:185:ARG:HB3	1:C:185:ARG:NH1	1.90	0.86
1:G:185:ARG:CG	1:G:188:ALA:HB3	2.07	0.85
2:B:1286:CYS:SG	2:B:1288:THR:HG22	2.15	0.85
2:D:1409:THR:HG23	2:D:1410:THR:HG23	1.58	0.82
1:G:432:GLU:HG2	2:H:1442:SER:H	1.46	0.81
1:C:185:ARG:HH11	1:C:185:ARG:CB	1.92	0.81
1:A:227:LEU:HD23	1:A:301:VAL:HB	1.63	0.80
1:A:393:LEU:HD23	1:A:394:LEU:N	1.96	0.80
1:C:244:LEU:O	1:C:246:PRO:HD3	1.80	0.80
1:G:432:GLU:HG3	2:H:1442:SER:HB2	1.62	0.80
1:C:166:ASN:H	1:C:166:ASN:HD22	0.81	0.79
2:B:1414:LYS:HG3	2:B:1415:ASP:N	1.96	0.79
1:C:185:ARG:HB2	1:C:188:ALA:HB3	1.63	0.79
2:H:1331:ILE:O	2:H:1335:ARG:HG3	1.82	0.79
1:G:198:CYS:H	1:G:199:PRO:CD	1.71	0.79
2:H:1414:LYS:HG3	2:H:1415:ASP:N	1.97	0.79
1:A:516:GLU:O	1:A:517:ASP:HB2	1.83	0.79
1:C:516:GLU:O	1:C:517:ASP:HB2	1.82	0.78
2:H:1271:GLU:HG2	2:H:1274:ARG:HH21	1.49	0.78
1:C:156:THR:HG22	1:C:157:PRO:N	1.97	0.78
2:F:1376:LYS:O	2:F:1376:LYS:HD3	1.82	0.78
2:F:1331:ILE:O	2:F:1335:ARG:HG3	1.83	0.78
1:G:292:LYS:H	1:G:292:LYS:HD3	1.47	0.78
1:G:199:PRO:HG2	1:G:200:GLU:H	1.49	0.77
1:A:339:GLN:HG2	1:A:577:ARG:NH2	1.98	0.76
1:G:185:ARG:HD2	1:G:373:ASP:OD2	1.85	0.76
2:F:1412:HIS:HD2	2:F:1413:GLU:H	1.32	0.76
1:E:516:GLU:O	1:E:517:ASP:HB2	1.86	0.76
2:H:1410:THR:HG22	2:H:1412:HIS:H	1.51	0.76
1:C:407:ARG:HH11	1:C:407:ARG:HG3	1.51	0.75
2:D:1414:LYS:NZ	2:D:1418:LYS:HD3	2.00	0.75
1:G:516:GLU:O	1:G:517:ASP:HB2	1.84	0.75
1:E:386:HIS:HD2	1:E:388:GLN:H	1.34	0.75
1:G:209:MET:O	1:G:209:MET:HG2	1.86	0.75
1:A:160:LYS:H	1:A:160:LYS:CD	2.00	0.73
1:A:271:ILE:HD12	1:A:271:ILE:C	2.08	0.73
2:D:1402:GLU:O	2:D:1406:GLU:HG2	1.86	0.73
2:F:1313:ILE:HD13	2:F:1313:ILE:N	2.03	0.73
1:A:313:LYS:HB2	1:A:313:LYS:NZ	2.03	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1307:LEU:HD11	2:B:1326:LEU:HD11	1.71	0.73
2:B:1411:ASP:HA	2:B:1414:LYS:HG2	1.69	0.73
1:G:292:LYS:HD3	1:G:292:LYS:N	2.03	0.73
1:G:300:GLN:HG2	1:G:302:VAL:HG13	1.69	0.73
1:E:276:ARG:HD2	1:G:277:GLU:O	1.89	0.73
1:C:246:PRO:HG3	1:C:311:GLY:CA	2.19	0.72
1:C:407:ARG:HH22	1:C:444:ASP:CG	1.92	0.72
2:B:1414:LYS:HG3	2:B:1415:ASP:H	1.50	0.72
1:E:164:ARG:HG3	1:E:164:ARG:NH1	1.94	0.72
1:G:284:ILE:HD12	1:G:285:PRO:O	1.90	0.71
2:H:1280:LYS:HB3	2:H:1289:GLU:OE1	1.90	0.71
2:B:1360:LEU:HD12	2:B:1361:PRO:HD2	1.71	0.71
1:C:152:SER:HB3	1:C:153:PRO:CD	2.19	0.71
2:H:1307:LEU:HD11	2:H:1326:LEU:HD11	1.72	0.71
2:B:1268:THR:HB	2:B:1271:GLU:CD	2.10	0.70
2:F:1396:ARG:NH1	2:F:1434:LYS:HE2	2.05	0.70
1:G:271:ILE:HD12	1:G:272:LEU:N	2.07	0.70
1:G:506:ARG:HG2	1:G:506:ARG:HH11	1.56	0.70
1:C:312:ARG:NH1	1:C:313:LYS:HD2	2.06	0.70
1:G:175:GLY:C	1:G:177:ALA:H	1.95	0.70
1:G:185:ARG:HG2	1:G:188:ALA:HB3	1.73	0.70
2:F:1416:LYS:NZ	2:F:1416:LYS:HB3	2.07	0.69
2:F:1294:ASN:HD22	2:F:1296:PHE:H	1.38	0.69
2:B:1268:THR:HB	2:B:1271:GLU:CG	2.23	0.69
2:H:1268:THR:HB	2:H:1271:GLU:OE1	1.92	0.69
1:C:166:ASN:ND2	1:C:166:ASN:N	2.22	0.69
2:F:1268:THR:HG22	2:F:1271:GLU:CG	2.22	0.69
2:B:1271:GLU:O	2:B:1274:ARG:HG2	1.93	0.68
1:A:409:ILE:O	1:A:413:THR:HG22	1.93	0.68
2:F:1412:HIS:HD2	2:F:1413:GLU:N	1.92	0.68
1:C:369:HIS:HD2	1:C:370:ASP:OD1	1.76	0.68
1:C:156:THR:HG23	1:C:159:GLN:CB	2.24	0.68
1:C:332:GLU:OE2	1:C:332:GLU:HA	1.94	0.68
1:C:292:LYS:H	1:C:292:LYS:HD2	1.58	0.68
2:F:1280:LYS:HG2	2:F:1291:ILE:HG12	1.76	0.68
1:A:160:LYS:HE3	1:A:160:LYS:N	2.06	0.68
1:A:446:SER:O	1:A:450:LYS:HG3	1.94	0.68
1:G:207:LYS:HB2	1:G:207:LYS:NZ	2.08	0.67
2:D:1349:GLU:HG2	2:D:1378:THR:O	1.94	0.67
1:C:196:LEU:HD23	1:C:197:GLY:H	1.58	0.67
2:D:1376:LYS:O	2:D:1376:LYS:HD3	1.95	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:200:GLU:HG2	1:C:528:TYR:CG	2.28	0.67
1:A:313:LYS:HE2	2:F:1313:ILE:HB	1.75	0.67
1:A:386:HIS:HD2	1:A:388:GLN:H	1.42	0.67
1:A:477:LEU:HD11	1:A:540:ILE:HD13	1.77	0.67
2:F:1292:TYR:CE2	2:F:1307:LEU:HD12	2.29	0.67
2:F:1441:LEU:O	2:F:1441:LEU:HG	1.95	0.67
1:G:160:LYS:NZ	1:G:566:GLN:NE2	2.43	0.66
1:C:196:LEU:CD2	1:C:197:GLY:H	2.08	0.66
2:F:1294:ASN:ND2	2:F:1296:PHE:H	1.93	0.66
1:C:275:ASP:OD2	1:C:278:HIS:ND1	2.26	0.66
1:C:403:LYS:NZ	1:E:407:ARG:HH22	1.94	0.66
1:A:185:ARG:HB3	1:A:188:ALA:HB3	1.78	0.66
1:A:477:LEU:HD21	1:A:499:LEU:HD21	1.78	0.66
1:G:178:GLN:HG3	1:G:575:TYR:CE2	2.30	0.66
1:G:175:GLY:O	1:G:177:ALA:N	2.29	0.66
1:A:388:GLN:HB3	1:A:393:LEU:CD2	2.26	0.66
2:F:1268:THR:CG2	2:F:1271:GLU:HG2	2.24	0.66
1:E:477:LEU:HD11	1:E:540:ILE:HD13	1.78	0.65
1:C:194:LYS:HE3	4:C:618:HOH:O	1.96	0.65
1:G:207:LYS:HE2	1:G:524:SER:OG	1.97	0.65
2:B:1331:ILE:HG23	2:B:1440:PHE:HZ	1.60	0.65
2:B:1417:LEU:HD13	2:B:1421:PHE:CD1	2.30	0.65
1:C:292:LYS:HD2	1:C:292:LYS:N	2.11	0.65
1:E:446:SER:HB2	1:E:448:GLU:HG2	1.77	0.65
1:G:164:ARG:HG2	1:G:164:ARG:HH11	1.61	0.65
1:G:185:ARG:HG3	1:G:185:ARG:HH11	1.61	0.65
2:D:1294:ASN:HD22	2:D:1296:PHE:H	1.42	0.65
2:B:1307:LEU:HD23	2:B:1320:LEU:HD23	1.78	0.65
1:A:506:ARG:HG2	1:A:506:ARG:NH1	2.06	0.65
1:G:178:GLN:HG3	1:G:575:TYR:HE2	1.60	0.65
2:H:1413:GLU:HA	2:H:1416:LYS:HE3	1.78	0.64
1:C:446:SER:O	1:C:450:LYS:HG3	1.96	0.64
1:G:446:SER:HB2	1:G:448:GLU:HG2	1.77	0.64
1:E:297:PHE:CD1	1:E:480:LEU:HD11	2.32	0.64
2:F:1345:TRP:CE3	2:F:1358:ARG:HG3	2.33	0.64
1:A:386:HIS:CD2	1:A:388:GLN:H	2.16	0.64
2:D:1313:ILE:HD12	2:D:1313:ILE:N	2.10	0.64
1:C:480:LEU:HD23	1:C:498:ILE:HG23	1.80	0.64
2:F:1412:HIS:CD2	2:F:1413:GLU:H	2.16	0.64
2:H:1391:GLN:CA	2:H:1391:GLN:HE21	2.11	0.64
1:C:386:HIS:HD2	1:C:388:GLN:H	1.46	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:432:GLU:HG3	2:H:1442:SER:CB	2.28	0.63
1:A:313:LYS:HE2	2:F:1313:ILE:CG2	2.28	0.63
1:C:227:LEU:HD23	1:C:301:VAL:HB	1.80	0.63
1:C:169:GLU:HB3	1:C:597:ARG:HD2	1.79	0.63
1:E:185:ARG:HB3	1:E:188:ALA:HB3	1.81	0.62
1:C:308:ASN:HD21	1:C:311:GLY:HA2	1.62	0.62
2:D:1409:THR:HG23	2:D:1410:THR:N	2.14	0.62
2:H:1307:LEU:HD11	2:H:1326:LEU:CD1	2.29	0.62
1:C:476:LEU:HD21	1:C:502:ILE:HG12	1.82	0.62
1:C:223:LYS:HE3	4:C:641:HOH:O	1.99	0.62
2:B:1331:ILE:HG23	2:B:1440:PHE:CZ	2.35	0.62
1:C:156:THR:CG2	1:C:159:GLN:HB3	2.29	0.62
1:C:221:THR:HG21	1:C:276:ARG:HB3	1.81	0.62
1:G:506:ARG:HG2	1:G:506:ARG:NH1	2.14	0.62
1:C:358:ASP:OD1	2:F:1424:PRO:HD2	1.99	0.62
1:A:285:PRO:HG2	1:A:313:LYS:HZ2	1.65	0.62
1:A:495:PHE:HB2	1:A:549:LYS:HE3	1.80	0.62
1:C:372:PRO:O	1:C:418:SER:HB3	2.00	0.62
1:G:586:ARG:HG3	1:G:586:ARG:HH11	1.63	0.62
1:A:313:LYS:HB2	1:A:313:LYS:HZ3	1.63	0.61
1:A:476:LEU:HD11	1:A:510:PRO:HD2	1.82	0.61
1:C:308:ASN:ND2	1:C:311:GLY:HA2	2.15	0.61
1:A:587:GLN:HE21	1:A:587:GLN:HA	1.64	0.61
1:C:157:PRO:O	1:C:158:SER:HB2	1.98	0.61
2:F:1348:CYS:SG	2:F:1377:ALA:HB3	2.41	0.61
1:G:185:ARG:HG3	1:G:188:ALA:HB3	1.81	0.61
1:G:275:ASP:OD2	1:G:278:HIS:ND1	2.29	0.61
1:C:407:ARG:HG3	1:C:407:ARG:NH1	2.15	0.61
2:B:1316:LYS:HE3	2:B:1316:LYS:O	2.00	0.61
1:C:209:MET:HA	2:D:1443:ARG:HG3	1.82	0.61
2:H:1340:LYS:HG2	2:H:1383:TYR:CD2	2.36	0.61
2:F:1307:LEU:HB3	2:F:1320:LEU:CD2	2.31	0.61
1:G:292:LYS:H	1:G:292:LYS:CD	2.07	0.61
1:G:495:PHE:HB2	1:G:549:LYS:HE3	1.82	0.61
1:C:182:TRP:HE1	1:C:594:GLN:NE2	1.99	0.61
2:H:1307:LEU:C	2:H:1319:PRO:HG2	2.21	0.61
2:B:1280:LYS:HD3	2:B:1289:GLU:OE2	1.99	0.60
1:G:347:GLY:O	1:G:561:ARG:HG3	2.01	0.60
1:G:216:ILE:HG21	4:G:613:HOH:O	2.00	0.60
1:A:424:PRO:O	1:A:458:GLU:HG3	2.01	0.60
1:C:209:MET:HA	2:D:1443:ARG:CG	2.32	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:1340:LYS:HD2	2:F:1383:TYR:CD2	2.37	0.60
2:F:1412:HIS:CD2	2:F:1413:GLU:N	2.69	0.60
1:A:394:LEU:HD13	1:A:401:ILE:CD1	2.32	0.59
1:G:586:ARG:HG3	1:G:586:ARG:NH1	2.17	0.59
1:A:500:LYS:HE3	1:A:552:LEU:HD21	1.83	0.59
1:C:312:ARG:HH11	1:C:313:LYS:HB3	1.66	0.59
1:E:164:ARG:HE	1:E:167:ARG:NH2	2.00	0.59
1:A:182:TRP:CE3	1:A:573:ARG:HD3	2.37	0.59
1:E:308:ASN:ND2	1:E:313:LYS:O	2.34	0.59
1:G:209:MET:CB	2:H:1443:ARG:HB3	2.20	0.59
1:C:156:THR:HG23	1:C:159:GLN:HB2	1.84	0.59
1:C:500:LYS:HE3	1:C:552:LEU:HD21	1.85	0.59
2:D:1313:ILE:H	2:D:1313:ILE:CD1	2.12	0.59
1:C:156:THR:HG23	1:C:159:GLN:HB3	1.83	0.59
1:C:200:GLU:HG2	1:C:528:TYR:CD1	2.38	0.59
1:G:164:ARG:HG2	1:G:164:ARG:NH1	2.18	0.59
1:G:311:GLY:O	1:G:312:ARG:HD2	2.02	0.59
2:H:1414:LYS:CG	2:H:1415:ASP:N	2.65	0.59
1:E:307:ILE:CG2	1:E:309:THR:HG23	2.32	0.59
2:B:1286:CYS:HB3	2:B:1315:CYS:SG	2.43	0.58
1:C:156:THR:N	1:C:157:PRO:CD	2.66	0.58
2:D:1268:THR:HG23	2:D:1271:GLU:HG2	1.85	0.58
1:A:160:LYS:HZ2	1:A:566:GLN:HB3	1.68	0.58
1:A:394:LEU:HD13	1:A:401:ILE:HD12	1.85	0.58
1:E:212:LYS:HB2	1:E:215:ASP:OD2	2.03	0.58
1:C:495:PHE:CE1	1:C:544:LEU:HD13	2.38	0.58
1:G:426:LEU:HD11	1:G:518:MET:HE3	1.84	0.58
2:B:1277:GLU:OE2	2:B:1336:ARG:NH2	2.37	0.58
1:E:386:HIS:CD2	1:E:388:GLN:H	2.18	0.58
2:H:1366:ARG:HG3	2:H:1366:ARG:HH11	1.69	0.58
1:A:495:PHE:CE1	1:A:544:LEU:HD13	2.39	0.58
2:F:1307:LEU:HB3	2:F:1320:LEU:HD21	1.86	0.58
1:E:564:LYS:HD3	1:E:569:GLY:HA2	1.86	0.58
2:B:1340:LYS:HD3	2:B:1383:TYR:CG	2.39	0.57
1:C:223:LYS:NZ	1:C:256:GLN:HE21	2.02	0.57
1:C:321:GLU:HA	4:C:661:HOH:O	2.04	0.57
1:G:334:ASP:HA	1:G:337:PHE:CE2	2.38	0.57
1:A:243:LEU:HD22	1:A:253:LEU:HD13	1.87	0.57
1:G:271:ILE:HD13	1:G:283:GLN:HB3	1.85	0.57
1:G:396:SER:OG	1:G:401:ILE:HD11	2.04	0.57
1:A:307:ILE:HA	4:A:614:HOH:O	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:579:PRO:HG3	1:C:587:GLN:HB3	1.87	0.57
2:D:1268:THR:HG23	2:D:1271:GLU:CD	2.25	0.57
2:H:1320:LEU:HD21	2:H:1426:VAL:HG22	1.85	0.57
1:A:313:LYS:HE2	2:F:1313:ILE:CB	2.34	0.57
2:D:1277:GLU:OE2	2:D:1336:ARG:NH2	2.37	0.56
1:C:447:ARG:O	1:C:447:ARG:NE	2.38	0.56
1:C:292:LYS:HG2	1:C:293:GLU:N	2.20	0.56
1:C:292:LYS:H	1:C:292:LYS:CD	2.18	0.56
1:E:170:VAL:HG13	1:E:594:GLN:HG2	1.87	0.56
1:E:508:TYR:CE2	1:E:531:LEU:HD23	2.41	0.56
1:C:297:PHE:CD1	1:C:480:LEU:HD11	2.41	0.56
2:D:1340:LYS:HD3	2:D:1383:TYR:CD2	2.41	0.56
1:E:157:PRO:HB3	1:E:354:SER:HB3	1.87	0.56
1:A:579:PRO:HG3	1:A:587:GLN:HB3	1.88	0.56
1:G:308:ASN:ND2	1:G:311:GLY:HA2	2.21	0.56
2:B:1294:ASN:HD22	2:B:1296:PHE:H	1.53	0.56
1:G:292:LYS:HE2	1:G:293:GLU:H	1.70	0.55
1:E:338:GLU:HG2	1:E:339:GLN:N	2.21	0.55
2:H:1350:GLU:OE2	2:H:1351:PRO:HD2	2.05	0.55
1:C:343:LEU:HD23	1:C:344:VAL:N	2.21	0.55
1:A:448:GLU:HA	1:A:448:GLU:OE1	2.06	0.55
1:G:221:THR:O	1:G:225:GLU:HG3	2.06	0.55
1:G:237:ILE:HD12	1:G:252:THR:HG21	1.89	0.55
1:G:426:LEU:HD21	1:G:435:TYR:HB2	1.88	0.55
1:C:386:HIS:CD2	1:C:388:GLN:H	2.23	0.55
1:E:394:LEU:HD12	1:E:398:PHE:HE1	1.72	0.55
1:A:157:PRO:C	1:A:159:GLN:H	1.96	0.55
1:A:160:LYS:CD	1:A:160:LYS:N	2.70	0.55
1:A:313:LYS:CE	2:F:1313:ILE:HB	2.36	0.55
1:E:495:PHE:HB2	1:E:549:LYS:HE3	1.89	0.55
2:B:1281:CYS:SG	2:B:1326:LEU:HD23	2.47	0.54
1:G:157:PRO:O	1:G:158:SER:HB2	2.05	0.54
1:G:297:PHE:CE1	1:G:300:GLN:HB2	2.42	0.54
2:H:1330:LEU:O	2:H:1334:ILE:HG13	2.06	0.54
1:G:160:LYS:HZ2	1:G:566:GLN:HE21	1.55	0.54
1:G:185:ARG:CD	1:G:373:ASP:OD2	2.55	0.54
1:C:540:ILE:HD12	1:C:540:ILE:H	1.72	0.54
1:A:407:ARG:HG3	1:A:407:ARG:HH11	1.72	0.54
1:A:344:VAL:HG11	1:A:539:ILE:HG21	1.90	0.54
1:A:388:GLN:HB3	1:A:393:LEU:HD21	1.90	0.54
1:C:312:ARG:HH11	1:C:313:LYS:HD2	1.71	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:582:ASP:OD1	1:E:583:GLY:N	2.40	0.54
1:C:325:LEU:HD21	1:C:506:ARG:HD3	1.90	0.54
1:G:341:MET:HG3	1:G:575:TYR:CE1	2.42	0.54
2:B:1331:ILE:O	2:B:1335:ARG:HG3	2.07	0.54
2:D:1409:THR:HG23	2:D:1410:THR:H	1.71	0.54
2:F:1345:TRP:CZ3	2:F:1358:ARG:HG3	2.43	0.54
1:E:217:ARG:HD2	2:F:1364:PHE:CE1	2.43	0.54
1:A:182:TRP:CZ2	1:A:594:GLN:HG3	2.43	0.54
1:A:202:LEU:C	1:A:202:LEU:HD23	2.28	0.54
1:A:445:LEU:HD22	1:A:449:ASP:HB3	1.90	0.54
1:A:388:GLN:HB3	1:A:393:LEU:HD22	1.88	0.53
1:C:223:LYS:HZ3	1:C:256:GLN:NE2	2.06	0.53
2:H:1337:PHE:HE2	2:H:1395:TYR:CE2	2.26	0.53
2:H:1413:GLU:HA	2:H:1416:LYS:CE	2.37	0.53
2:F:1307:LEU:O	2:F:1320:LEU:HG	2.08	0.53
1:C:194:LYS:O	1:C:462:LEU:HD12	2.08	0.53
2:D:1268:THR:HG23	2:D:1271:GLU:CG	2.38	0.53
2:B:1415:ASP:HA	2:B:1418:LYS:HB3	1.90	0.53
1:E:222:CYS:O	1:E:226:GLU:HB2	2.09	0.53
1:C:180:VAL:HG12	1:C:180:VAL:O	2.09	0.53
1:C:213:LEU:HB2	1:C:214:PRO:HD3	1.91	0.53
2:F:1281:CYS:SG	2:F:1326:LEU:HD23	2.49	0.53
1:G:275:ASP:CG	1:G:278:HIS:HD1	2.12	0.53
1:A:182:TRP:CD2	1:A:573:ARG:HD3	2.43	0.53
1:C:221:THR:HG22	1:C:225:GLU:OE2	2.09	0.53
1:G:199:PRO:CG	1:G:200:GLU:H	2.19	0.53
2:B:1308:TYR:CD1	2:B:1308:TYR:C	2.82	0.53
2:B:1438:GLU:OE1	2:B:1438:GLU:N	2.42	0.53
1:G:185:ARG:HB3	1:G:185:ARG:CZ	2.39	0.52
1:G:354:SER:HB2	1:G:356:THR:HG23	1.91	0.52
1:C:201:ALA:HA	1:C:439:PRO:CD	2.39	0.52
2:F:1415:ASP:HA	2:F:1418:LYS:HB3	1.89	0.52
1:A:477:LEU:HD21	1:A:499:LEU:CD2	2.40	0.52
1:E:427:ARG:HD3	4:E:616:HOH:O	2.08	0.52
1:G:300:GLN:HG2	1:G:302:VAL:CG1	2.38	0.52
1:C:182:TRP:HE1	1:C:594:GLN:HE22	1.58	0.52
1:G:586:ARG:HH11	1:G:586:ARG:CG	2.23	0.52
2:B:1410:THR:HG23	2:B:1413:GLU:HB3	1.92	0.52
1:G:209:MET:HE2	2:H:1444:SER:HB2	1.92	0.52
1:C:295:SER:O	1:C:296:LEU:HD23	2.09	0.52
2:D:1376:LYS:HE2	2:D:1376:LYS:CA	2.33	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:1307:LEU:HD23	2:F:1320:LEU:HD23	1.92	0.52
1:G:294:TYR:CD1	1:G:487:SER:HB3	2.44	0.52
1:C:196:LEU:CD1	1:C:468:ILE:HD12	2.39	0.52
1:A:222:CYS:O	1:A:226:GLU:HB2	2.09	0.52
1:A:285:PRO:HG2	1:A:313:LYS:NZ	2.25	0.52
2:B:1307:LEU:HD11	2:B:1326:LEU:CD1	2.37	0.51
1:A:570:THR:HG22	1:A:597:ARG:HA	1.92	0.51
2:B:1276:CYS:SG	2:B:1390:THR:HG22	2.49	0.51
2:D:1416:LYS:HD2	2:D:1416:LYS:C	2.31	0.51
2:F:1347:ILE:CD1	2:F:1356:ARG:HB2	2.40	0.51
2:H:1307:LEU:HD12	2:H:1319:PRO:HB2	1.92	0.51
1:A:192:SER:OG	1:A:194:LYS:HE3	2.09	0.51
2:B:1400:ASP:HA	2:B:1434:LYS:HD2	1.93	0.51
1:G:478:PHE:CD1	1:G:544:LEU:HD11	2.45	0.51
2:H:1413:GLU:CA	2:H:1416:LYS:HE3	2.41	0.51
1:A:343:LEU:C	1:A:343:LEU:HD23	2.30	0.51
2:B:1394:PHE:O	2:B:1398:ILE:HG23	2.11	0.51
1:G:207:LYS:HB2	1:G:207:LYS:HZ3	1.75	0.51
1:G:574:LEU:HD12	1:G:574:LEU:N	2.25	0.51
1:A:393:LEU:HD23	1:A:393:LEU:C	2.30	0.51
1:A:509:TYR:CE2	1:A:518:MET:SD	3.04	0.51
2:B:1330:LEU:HD11	2:B:1399:PHE:CE2	2.46	0.51
1:E:447:ARG:HH11	1:E:447:ARG:HB3	1.75	0.51
1:A:362:ASP:O	1:A:366:VAL:HG23	2.11	0.51
1:G:160:LYS:NZ	1:G:566:GLN:HE21	2.09	0.51
1:G:494:ARG:NH1	1:G:494:ARG:HG3	2.25	0.51
2:H:1391:GLN:HE21	2:H:1391:GLN:C	2.13	0.51
1:A:160:LYS:NZ	1:A:566:GLN:HB3	2.26	0.51
2:D:1408:LEU:HD12	2:D:1413:GLU:OE1	2.10	0.51
1:G:307:ILE:HG23	1:G:309:THR:HG23	1.93	0.51
1:G:510:PRO:HA	4:G:607:HOH:O	2.11	0.51
1:A:339:GLN:HG2	1:A:577:ARG:CZ	2.41	0.50
2:B:1270:GLU:CD	2:B:1270:GLU:C	2.69	0.50
1:C:402:PHE:CD1	1:C:430:HIS:CE1	2.99	0.50
2:D:1414:LYS:HZ1	2:D:1418:LYS:HD3	1.74	0.50
2:F:1363:GLN:NE2	2:F:1370:LEU:HD23	2.26	0.50
1:A:360:LEU:HD11	1:A:409:ILE:HD11	1.93	0.50
1:C:494:ARG:HG3	1:C:494:ARG:NH1	2.26	0.50
1:E:202:LEU:HD12	2:H:1364:PHE:HB3	1.92	0.50
1:E:583:GLY:O	1:E:585:GLU:N	2.45	0.50
1:G:271:ILE:HD12	1:G:271:ILE:C	2.32	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:368:ASN:O	1:G:371:ARG:HG2	2.11	0.50
1:A:211:GLN:HG2	4:A:611:HOH:O	2.10	0.50
1:G:207:LYS:HD3	2:H:1443:ARG:NH1	2.26	0.50
1:G:578:ARG:HG3	1:G:578:ARG:HH11	1.76	0.50
1:E:308:ASN:HD21	1:E:313:LYS:H	1.58	0.50
1:E:368:ASN:O	1:E:371:ARG:HG2	2.11	0.50
2:H:1435:ASN:O	2:H:1439:GLN:HB2	2.11	0.50
1:G:334:ASP:HA	1:G:337:PHE:CD2	2.47	0.50
1:E:170:VAL:CG1	1:E:594:GLN:HG2	2.42	0.50
1:G:210:PHE:HE1	2:H:1388:LEU:HD23	1.76	0.50
1:C:583:GLY:O	1:C:585:GLU:N	2.44	0.50
1:E:363:LEU:O	1:E:367:ILE:HG13	2.11	0.50
1:G:446:SER:HB3	1:G:448:GLU:OE2	2.12	0.50
2:D:1320:LEU:HD13	2:D:1320:LEU:O	2.12	0.50
1:G:305:GLU:HB3	1:G:318:LYS:HB3	1.93	0.50
1:G:391:ASN:HB2	1:G:393:LEU:HG	1.94	0.49
2:H:1414:LYS:NZ	2:H:1418:LYS:NZ	2.60	0.49
1:A:157:PRO:HB3	1:A:354:SER:HB3	1.94	0.49
1:A:200:GLU:OE2	1:A:203:THR:HG22	2.12	0.49
1:E:307:ILE:HG22	4:E:602:HOH:O	2.11	0.49
1:G:175:GLY:C	1:G:177:ALA:N	2.64	0.49
1:G:432:GLU:CG	2:H:1442:SER:H	2.22	0.49
2:H:1366:ARG:HG3	2:H:1366:ARG:NH1	2.27	0.49
1:C:407:ARG:NH2	1:C:444:ASP:OD2	2.45	0.49
1:E:503:LEU:HD22	1:E:534:THR:HG23	1.94	0.49
1:G:221:THR:HG21	1:G:276:ARG:HB2	1.94	0.49
1:G:448:GLU:HG2	1:G:449:ASP:H	1.77	0.49
1:A:191:ILE:HD13	1:A:191:ILE:O	2.11	0.49
1:C:253:LEU:HD12	1:C:314:LEU:HD22	1.95	0.49
1:G:185:ARG:CG	1:G:185:ARG:HH11	2.24	0.49
1:G:583:GLY:O	1:G:585:GLU:N	2.45	0.49
2:H:1346:LEU:HD23	2:H:1381:PRO:HA	1.94	0.49
1:G:494:ARG:HG3	1:G:494:ARG:HH11	1.77	0.49
1:A:586:ARG:HG3	1:A:586:ARG:NH1	2.28	0.49
1:E:358:ASP:HB2	1:E:359:PRO:HD3	1.95	0.49
1:E:547:PHE:CD1	1:E:547:PHE:C	2.86	0.49
2:H:1281:CYS:SG	2:H:1326:LEU:HD23	2.53	0.49
1:A:339:GLN:HG2	1:A:577:ARG:HH21	1.77	0.49
1:C:237:ILE:HD13	1:C:252:THR:HG21	1.95	0.49
1:E:338:GLU:HG2	1:E:339:GLN:H	1.75	0.49
2:H:1420:GLN:HB3	2:H:1421:PHE:CD1	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:1294:ASN:HD22	2:F:1296:PHE:N	2.10	0.49
1:G:221:THR:HG22	1:G:225:GLU:CD	2.34	0.49
1:G:308:ASN:HD21	1:G:311:GLY:HA2	1.78	0.49
1:G:385:LYS:HE2	1:G:427:ARG:HD2	1.94	0.49
1:A:213:LEU:HG	4:A:627:HOH:O	2.13	0.48
2:B:1437:ALA:HB3	2:B:1438:GLU:OE1	2.13	0.48
2:H:1297:ASP:HB2	2:H:1306:SER:OG	2.13	0.48
1:A:313:LYS:HE2	2:F:1313:ILE:HG21	1.94	0.48
1:C:275:ASP:CG	1:C:278:HIS:HD1	2.15	0.48
1:C:285:PRO:HD2	1:C:312:ARG:O	2.13	0.48
1:C:343:LEU:HD23	1:C:343:LEU:C	2.33	0.48
1:C:296:LEU:HA	1:C:300:GLN:OE1	2.14	0.48
2:H:1345:TRP:CE3	2:H:1358:ARG:HG3	2.49	0.48
2:D:1415:ASP:HA	2:D:1418:LYS:HB3	1.95	0.48
1:A:586:ARG:HG3	1:A:586:ARG:HH11	1.77	0.48
1:C:201:ALA:HA	1:C:439:PRO:HD3	1.94	0.48
2:F:1416:LYS:HB3	2:F:1416:LYS:HZ2	1.78	0.48
2:D:1416:LYS:HG3	2:D:1417:LEU:N	2.27	0.48
2:H:1413:GLU:N	2:H:1416:LYS:HE3	2.28	0.48
1:C:152:SER:CB	1:C:153:PRO:CD	2.87	0.48
1:G:236:LYS:HD3	1:G:236:LYS:N	2.28	0.48
2:B:1308:TYR:C	2:B:1308:TYR:HD1	2.17	0.48
1:G:221:THR:HG22	1:G:225:GLU:OE2	2.13	0.48
2:H:1412:HIS:O	2:H:1416:LYS:CG	2.51	0.48
1:A:227:LEU:HD23	1:A:301:VAL:CB	2.37	0.48
2:B:1352:THR:O	2:B:1352:THR:HG22	2.14	0.48
1:E:360:LEU:HD11	1:E:409:ILE:HD11	1.96	0.48
1:E:447:ARG:HG2	1:E:448:GLU:N	2.28	0.48
2:F:1268:THR:HG22	2:F:1271:GLU:CD	2.34	0.48
1:G:311:GLY:C	1:G:312:ARG:HD2	2.34	0.48
1:A:307:ILE:CG2	1:A:309:THR:HG23	2.44	0.47
2:D:1286:CYS:SG	2:D:1288:THR:HG23	2.54	0.47
1:A:297:PHE:CG	1:A:480:LEU:HD11	2.49	0.47
1:A:583:GLY:O	1:A:585:GLU:N	2.47	0.47
1:E:164:ARG:NE	1:E:167:ARG:NH2	2.62	0.47
1:E:321:GLU:HB2	4:E:635:HOH:O	2.12	0.47
1:C:152:SER:CB	1:C:153:PRO:HD2	2.29	0.47
1:C:199:PRO:O	1:C:200:GLU:HB2	2.14	0.47
1:C:313:LYS:HG2	1:C:314:LEU:N	2.29	0.47
1:E:243:LEU:HD22	1:E:253:LEU:HD13	1.96	0.47
1:E:512:TYR:HA	1:E:513:PRO:C	2.33	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:1420:GLN:HE21	2:H:1420:GLN:C	2.17	0.47
1:E:182:TRP:HE1	1:E:594:GLN:HE22	1.63	0.47
2:H:1286:CYS:HB3	2:H:1315:CYS:HB2	1.95	0.47
1:A:333:GLU:H	1:A:333:GLU:CD	2.17	0.47
1:A:426:LEU:HD11	1:A:435:TYR:HB2	1.96	0.47
1:A:512:TYR:HA	1:A:513:PRO:C	2.35	0.47
2:B:1348:CYS:SG	2:B:1377:ALA:HB3	2.55	0.47
1:C:402:PHE:CE2	1:C:406:LEU:HD22	2.49	0.47
1:E:164:ARG:NH1	1:E:164:ARG:CG	2.67	0.47
2:F:1405:LEU:O	2:F:1414:LYS:HE2	2.14	0.47
1:G:160:LYS:NZ	1:G:566:GLN:HB2	2.30	0.47
1:G:382:LEU:HD23	1:G:382:LEU:HA	1.72	0.47
2:B:1428:GLN:HG2	2:B:1431:ARG:HH21	1.80	0.47
1:C:221:THR:CG2	1:C:276:ARG:H	2.28	0.47
2:F:1408:LEU:O	2:F:1414:LYS:HE3	2.15	0.47
1:G:271:ILE:HD12	1:G:272:LEU:C	2.35	0.47
1:A:266:ASN:HD22	2:F:1302:ASP:HA	1.80	0.46
1:A:363:LEU:O	1:A:367:ILE:HG13	2.15	0.46
1:E:157:PRO:N	1:E:159:GLN:OE1	2.48	0.46
1:E:445:LEU:HD22	1:E:449:ASP:HB3	1.95	0.46
1:G:237:ILE:HD11	1:G:320:TYR:CZ	2.50	0.46
1:A:191:ILE:HD11	1:A:193:LEU:HG	1.96	0.46
2:F:1408:LEU:HB2	2:F:1414:LYS:HG2	1.96	0.46
1:A:331:THR:HB	1:A:333:GLU:OE2	2.16	0.46
1:A:567:VAL:HG12	1:A:568:GLY:N	2.30	0.46
1:C:516:GLU:O	1:C:517:ASP:CB	2.56	0.46
1:E:476:LEU:HD21	1:E:510:PRO:HD2	1.97	0.46
1:A:307:ILE:HG23	1:A:309:THR:HG23	1.97	0.46
1:A:395:THR:HA	2:B:1325:GLN:NE2	2.31	0.46
1:A:514:PRO:O	2:B:1358:ARG:NH2	2.34	0.46
1:G:362:ASP:O	1:G:366:VAL:HG23	2.16	0.46
1:A:586:ARG:HH11	1:A:586:ARG:CG	2.29	0.46
1:C:223:LYS:NZ	1:C:256:GLN:NE2	2.64	0.46
1:E:202:LEU:HD12	2:H:1364:PHE:CB	2.46	0.46
1:E:297:PHE:CG	1:E:480:LEU:HD11	2.50	0.46
2:F:1416:LYS:HB3	2:F:1416:LYS:HZ3	1.81	0.46
2:H:1405:LEU:HD11	2:H:1422:PHE:CD2	2.51	0.46
1:C:157:PRO:O	1:C:158:SER:CB	2.64	0.46
1:G:343:LEU:HD23	1:G:344:VAL:N	2.30	0.46
2:H:1271:GLU:HG2	2:H:1274:ARG:NH2	2.25	0.46
2:D:1349:GLU:O	2:D:1351:PRO:HD3	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:1335:ARG:NH2	4:F:1607:HOH:O	2.49	0.46
1:C:305:GLU:HB3	1:C:318:LYS:HB3	1.97	0.46
1:A:232:LYS:HG3	1:A:237:ILE:HB	1.98	0.45
1:A:296:LEU:HA	1:A:300:GLN:OE1	2.16	0.45
2:B:1373:ALA:HB1	1:C:155:ALA:HB2	1.98	0.45
2:B:1307:LEU:HD23	2:B:1320:LEU:CD2	2.46	0.45
1:E:445:LEU:CD2	1:E:449:ASP:HB3	2.46	0.45
1:E:476:LEU:HD22	1:E:508:TYR:O	2.16	0.45
1:G:507:SER:HG	1:G:525:PHE:HZ	1.62	0.45
1:C:292:LYS:CG	1:C:293:GLU:N	2.79	0.45
1:C:480:LEU:HD12	1:C:511:LEU:HD13	1.98	0.45
2:D:1359:HIS:C	2:D:1359:HIS:CD2	2.90	0.45
1:E:382:LEU:HD13	1:E:429:VAL:CG1	2.47	0.45
1:G:476:LEU:HD22	1:G:508:TYR:O	2.16	0.45
1:A:446:SER:O	1:A:450:LYS:CG	2.63	0.45
2:D:1270:GLU:OE1	2:D:1270:GLU:C	2.55	0.45
2:D:1345:TRP:CE3	2:D:1356:ARG:HG2	2.52	0.45
1:E:166:ASN:HB3	1:E:597:ARG:HD2	1.98	0.45
1:E:213:LEU:HB2	1:E:214:PRO:HD3	1.99	0.45
1:G:182:TRP:HE1	1:G:594:GLN:NE2	2.15	0.45
2:H:1365:SER:HB3	2:H:1370:LEU:HD13	1.98	0.45
1:C:196:LEU:O	1:C:197:GLY:O	2.35	0.45
2:D:1348:CYS:SG	2:D:1377:ALA:HB3	2.56	0.45
1:E:406:LEU:O	1:E:410:ILE:HG13	2.16	0.45
1:G:161:TYR:O	1:G:164:ARG:NH1	2.49	0.45
1:G:194:LYS:O	1:G:462:LEU:HD12	2.16	0.45
1:G:542:SER:C	1:G:561:ARG:NH1	2.70	0.45
2:H:1310:CYS:CB	2:H:1315:CYS:SG	3.04	0.45
1:G:329:GLN:HE21	1:G:329:GLN:CA	2.29	0.45
1:A:157:PRO:C	1:A:159:GLN:N	2.64	0.45
1:A:161:TYR:O	1:A:164:ARG:HG2	2.17	0.45
2:D:1290:ASN:HD21	2:D:1310:CYS:HA	1.81	0.45
1:E:280:SER:O	2:F:1363:GLN:HG3	2.16	0.45
1:G:491:THR:HG23	1:G:492:SER:N	2.32	0.45
1:G:512:TYR:HA	1:G:513:PRO:C	2.36	0.45
2:H:1410:THR:HG22	2:H:1412:HIS:HB2	1.98	0.45
1:C:182:TRP:CZ3	1:C:575:TYR:CD2	3.05	0.45
1:A:160:LYS:N	1:A:160:LYS:HD3	2.32	0.45
1:A:586:ARG:HD2	1:A:586:ARG:HA	1.28	0.45
1:A:160:LYS:H	1:A:160:LYS:HD3	1.78	0.44
1:C:156:THR:N	1:C:157:PRO:HD2	2.31	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:166:ASN:HB2	1:C:597:ARG:CD	2.47	0.44
1:E:333:GLU:O	1:E:336:ASP:HB2	2.17	0.44
1:G:515:GLN:HE21	1:G:515:GLN:HB3	1.59	0.44
1:A:476:LEU:HD22	1:A:508:TYR:O	2.17	0.44
2:F:1440:PHE:HD1	2:F:1440:PHE:HA	1.66	0.44
1:G:222:CYS:O	1:G:226:GLU:HB2	2.17	0.44
1:G:547:PHE:CD1	1:G:547:PHE:C	2.91	0.44
2:H:1283:CYS:SG	2:H:1285:THR:OG1	2.75	0.44
2:H:1400:ASP:OD1	2:H:1403:CYS:HB2	2.17	0.44
2:B:1307:LEU:O	2:B:1319:PRO:HD2	2.17	0.44
1:C:164:ARG:HH11	1:C:167:ARG:HB2	1.81	0.44
2:F:1290:ASN:HD21	2:F:1310:CYS:HA	1.82	0.44
1:G:508:TYR:CE2	1:G:531:LEU:HD23	2.53	0.44
1:A:399:GLU:OE2	1:A:403:LYS:HE2	2.17	0.44
2:B:1396:ARG:NH1	2:B:1434:LYS:HE2	2.32	0.44
2:H:1348:CYS:SG	2:H:1377:ALA:HB3	2.57	0.44
2:H:1425:LYS:HD3	2:H:1429:ASP:OD2	2.17	0.44
1:A:212:LYS:HA	1:A:212:LYS:HD2	1.88	0.44
1:C:223:LYS:HZ1	1:C:256:GLN:HE21	1.65	0.44
1:C:403:LYS:NZ	1:E:407:ARG:NH2	2.62	0.44
2:F:1369:PRO:HG2	2:F:1379:LEU:HB2	1.99	0.44
2:H:1380:GLN:OE1	2:H:1380:GLN:HA	2.18	0.44
1:C:312:ARG:HD2	1:C:313:LYS:HB3	2.00	0.44
1:C:547:PHE:CD1	1:C:547:PHE:C	2.91	0.44
1:G:160:LYS:HZ1	1:G:566:GLN:NE2	2.14	0.44
1:G:297:PHE:CG	1:G:480:LEU:HD11	2.53	0.44
1:C:202:LEU:HD23	1:C:202:LEU:O	2.17	0.44
1:C:383:ASP:OD2	1:C:427:ARG:NH2	2.37	0.44
2:D:1316:LYS:HE2	2:D:1316:LYS:HB3	1.82	0.44
1:G:210:PHE:CE1	2:H:1388:LEU:HD23	2.51	0.44
1:G:476:LEU:HD13	1:G:509:TYR:CD1	2.52	0.44
1:G:476:LEU:HD13	1:G:509:TYR:HA	1.99	0.44
2:H:1280:LYS:HD3	2:H:1289:GLU:OE1	2.17	0.44
1:C:349:TYR:HB3	1:C:360:LEU:HB2	2.00	0.44
1:E:506:ARG:HG2	1:E:506:ARG:HH11	1.83	0.44
2:H:1286:CYS:SG	2:H:1288:THR:HG23	2.58	0.44
1:A:509:TYR:CE1	1:A:511:LEU:HB3	2.53	0.43
1:E:159:GLN:H	1:E:159:GLN:HG2	1.46	0.43
1:G:176:LEU:HG	1:G:176:LEU:O	2.17	0.43
1:A:180:VAL:HG23	1:A:180:VAL:O	2.17	0.43
2:B:1417:LEU:HD13	2:B:1421:PHE:HD1	1.78	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:494:ARG:HG3	1:C:494:ARG:HH11	1.83	0.43
2:F:1362:LEU:N	2:F:1362:LEU:CD1	2.81	0.43
2:H:1422:PHE:HB3	2:H:1427:LEU:HD21	1.99	0.43
1:A:193:LEU:CD2	1:A:464:ILE:HG12	2.48	0.43
1:A:445:LEU:HD22	1:A:449:ASP:CB	2.47	0.43
1:A:507:SER:HG	1:A:525:PHE:HZ	1.65	0.43
1:E:193:LEU:HD22	1:E:464:ILE:HG12	2.00	0.43
1:E:200:GLU:OE2	1:E:203:THR:HG22	2.18	0.43
2:H:1320:LEU:HD12	2:H:1320:LEU:O	2.17	0.43
1:C:166:ASN:HB2	1:C:597:ARG:HD3	2.01	0.43
1:C:260:ASP:OD1	1:C:260:ASP:C	2.57	0.43
1:C:221:THR:HG23	1:C:276:ARG:H	1.83	0.43
1:E:512:TYR:CD1	1:E:513:PRO:HA	2.53	0.43
2:H:1391:GLN:CA	2:H:1391:GLN:NE2	2.81	0.43
1:A:221:THR:HG21	1:A:276:ARG:HB3	1.99	0.43
1:C:512:TYR:HA	1:C:513:PRO:C	2.38	0.43
2:F:1286:CYS:HB3	2:F:1315:CYS:HB2	2.00	0.43
2:F:1313:ILE:H	2:F:1313:ILE:CD1	2.01	0.43
1:A:271:ILE:HD12	1:A:271:ILE:O	2.18	0.43
1:A:413:THR:HG21	1:A:420:LEU:HD11	2.01	0.43
2:B:1297:ASP:HB2	2:B:1306:SER:HA	2.00	0.43
1:C:284:ILE:O	1:C:284:ILE:HG13	2.19	0.43
2:D:1296:PHE:HZ	2:D:1405:LEU:CD1	2.32	0.43
2:F:1295:VAL:HG23	4:F:1603:HOH:O	2.18	0.43
1:G:227:LEU:HD23	1:G:301:VAL:HB	2.01	0.43
1:G:292:LYS:N	1:G:292:LYS:CD	2.72	0.43
1:C:210:PHE:HE1	2:D:1388:LEU:HD23	1.83	0.43
1:C:574:LEU:N	1:C:574:LEU:HD12	2.33	0.43
2:D:1394:PHE:O	2:D:1398:ILE:HG23	2.19	0.43
2:B:1268:THR:CG2	2:B:1271:GLU:HG2	2.50	0.42
1:C:394:LEU:HD12	1:C:398:PHE:HE1	1.83	0.42
2:D:1276:CYS:SG	2:D:1390:THR:HG22	2.58	0.42
1:G:586:ARG:HA	1:G:586:ARG:HD2	1.31	0.42
1:A:190:ASN:HD22	1:A:190:ASN:HA	1.56	0.42
1:A:578:ARG:HA	1:A:579:PRO:HD2	1.87	0.42
2:B:1284:PRO:HG2	2:B:1322:PHE:CG	2.54	0.42
1:E:201:ALA:HB3	2:H:1367:THR:C	2.39	0.42
1:G:176:LEU:O	1:G:177:ALA:O	2.38	0.42
1:G:402:PHE:CD1	1:G:430:HIS:CE1	3.07	0.42
1:G:285:PRO:HD2	1:G:312:ARG:O	2.20	0.42
1:A:388:GLN:CB	1:A:393:LEU:HD22	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:478:PHE:HD1	1:E:544:LEU:HD11	1.85	0.42
2:F:1427:LEU:HD23	2:F:1427:LEU:HA	1.84	0.42
1:G:292:LYS:HE2	1:G:293:GLU:N	2.34	0.42
2:H:1414:LYS:HZ2	2:H:1418:LYS:HZ1	1.67	0.42
1:A:458:GLU:HG3	1:A:473:SER:OG	2.20	0.42
1:C:202:LEU:HG	2:D:1442:SER:HB3	2.01	0.42
1:E:534:THR:O	4:E:637:HOH:O	2.21	0.42
2:F:1362:LEU:N	2:F:1362:LEU:HD12	2.34	0.42
2:H:1371:CYS:O	2:H:1374:CYS:O	2.38	0.42
1:A:495:PHE:O	1:A:499:LEU:HG	2.20	0.42
1:G:292:LYS:CE	1:G:293:GLU:H	2.31	0.42
2:H:1268:THR:HG22	2:H:1270:GLU:H	1.85	0.42
1:C:508:TYR:CZ	1:C:531:LEU:HD23	2.55	0.42
2:D:1335:ARG:HD3	4:D:1606:HOH:O	2.20	0.42
2:D:1350:GLU:OE2	2:D:1352:THR:HG23	2.20	0.42
1:E:243:LEU:HD23	1:E:243:LEU:N	2.35	0.42
1:G:385:LYS:HE2	1:G:427:ARG:CD	2.50	0.42
1:A:479:HIS:CG	1:A:515:GLN:HG3	2.54	0.42
1:A:508:TYR:CZ	1:A:531:LEU:HD23	2.55	0.42
1:A:516:GLU:O	1:A:517:ASP:CB	2.55	0.42
2:B:1316:LYS:HA	2:B:1316:LYS:HD2	1.64	0.42
2:B:1290:ASN:N	2:B:1290:ASN:HD22	2.18	0.42
2:D:1409:THR:CG2	2:D:1410:THR:N	2.82	0.42
2:F:1441:LEU:O	2:F:1441:LEU:CG	2.64	0.42
1:A:388:GLN:O	1:A:393:LEU:HD22	2.20	0.41
1:E:564:LYS:CD	1:E:569:GLY:HA2	2.49	0.41
1:G:360:LEU:HD11	1:G:409:ILE:HG12	2.00	0.41
1:G:364:ILE:HG23	1:G:413:THR:HG22	2.02	0.41
2:H:1391:GLN:HE21	2:H:1391:GLN:HA	1.85	0.41
1:A:343:LEU:HD23	1:A:344:VAL:N	2.35	0.41
1:A:410:ILE:HD13	1:A:445:LEU:HD21	2.01	0.41
1:C:479:HIS:CD2	1:C:515:GLN:NE2	2.88	0.41
1:E:567:VAL:HG12	1:E:568:GLY:N	2.35	0.41
1:A:360:LEU:O	1:A:364:ILE:HG13	2.19	0.41
1:A:522:TYR:HA	1:A:525:PHE:HB3	2.02	0.41
2:B:1360:LEU:HD11	2:B:1369:PRO:HG3	2.02	0.41
1:C:196:LEU:HD11	1:C:468:ILE:HD12	2.00	0.41
1:C:476:LEU:CD2	1:C:502:ILE:HG12	2.50	0.41
1:C:570:THR:HG22	1:C:597:ARG:HA	2.02	0.41
1:E:217:ARG:HD2	2:F:1364:PHE:CD1	2.54	0.41
1:G:249:GLU:H	1:G:249:GLU:CD	2.22	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:349:TYR:HB3	1:A:360:LEU:HB2	2.03	0.41
1:C:358:ASP:N	1:C:359:PRO:CD	2.83	0.41
2:D:1438:GLU:OE2	2:D:1441:LEU:HD12	2.20	0.41
1:G:349:TYR:HB3	1:G:360:LEU:HB2	2.02	0.41
1:G:567:VAL:HG12	1:G:568:GLY:N	2.35	0.41
1:A:386:HIS:HD2	1:A:388:GLN:N	2.12	0.41
1:E:288:LEU:HD22	1:E:291:LEU:HD12	2.02	0.41
1:E:300:GLN:NE2	1:E:302:VAL:HG12	2.35	0.41
2:H:1415:ASP:HA	2:H:1418:LYS:HB3	2.02	0.41
1:A:182:TRP:CD2	1:A:573:ARG:CD	3.03	0.41
1:A:323:VAL:HA	1:A:324:PRO:HD3	1.87	0.41
1:C:200:GLU:OE1	1:C:438:PRO:HA	2.20	0.41
2:H:1345:TRP:CZ3	2:H:1358:ARG:HG3	2.56	0.41
1:A:271:ILE:C	1:A:271:ILE:CD1	2.80	0.41
2:F:1354:ARG:HG2	2:F:1354:ARG:HH11	1.86	0.41
2:F:1396:ARG:HH12	2:F:1434:LYS:HE2	1.84	0.41
1:G:166:ASN:HB2	1:G:597:ARG:HD3	2.03	0.41
1:A:331:THR:CB	1:A:333:GLU:OE2	2.69	0.41
1:A:331:THR:OG1	1:A:334:ASP:OD1	2.38	0.41
1:A:352:SER:H	1:A:352:SER:HG	1.67	0.41
1:A:426:LEU:HD22	1:A:433:PRO:O	2.21	0.41
1:C:209:MET:CA	2:D:1443:ARG:HG3	2.49	0.41
2:D:1303:MET:HE2	2:D:1417:LEU:HD21	2.03	0.41
1:E:578:ARG:HA	1:E:579:PRO:HD3	1.85	0.41
1:A:164:ARG:HG2	1:A:164:ARG:HH11	1.86	0.41
1:A:334:ASP:HA	1:A:337:PHE:CD2	2.56	0.41
2:B:1416:LYS:O	2:B:1420:GLN:HB2	2.21	0.41
1:C:399:GLU:OE2	1:C:403:LYS:HE3	2.21	0.41
2:F:1348:CYS:SG	2:F:1377:ALA:CB	3.08	0.41
2:F:1351:PRO:HA	2:F:1354:ARG:HH11	1.86	0.41
1:G:270:VAL:HG21	1:G:288:LEU:HD11	2.01	0.41
2:H:1269:ASP:HA	2:H:1272:LYS:HG2	2.01	0.41
1:C:156:THR:N	1:C:157:PRO:HD3	2.36	0.41
2:D:1437:ALA:N	4:D:1601:HOH:O	2.52	0.41
2:B:1273:TYR:HB3	2:B:1394:PHE:CD1	2.56	0.40
2:D:1416:LYS:O	2:D:1420:GLN:HB2	2.21	0.40
1:G:192:SER:C	1:G:193:LEU:HD23	2.42	0.40
1:G:344:VAL:HG11	1:G:539:ILE:HG21	2.03	0.40
1:A:387:GLU:O	1:A:391:ASN:ND2	2.54	0.40
1:A:536:ASP:OD1	1:A:586:ARG:NH2	2.54	0.40
2:D:1340:LYS:HD3	2:D:1383:TYR:CG	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:207:LYS:HG2	1:E:208:SER:N	2.36	0.40
1:G:423:VAL:HA	1:G:424:PRO:HD3	1.91	0.40
1:G:160:LYS:HZ2	1:G:566:GLN:HB2	1.85	0.40
1:G:426:LEU:HD11	1:G:518:MET:CE	2.50	0.40
2:D:1405:LEU:HA	2:D:1408:LEU:HD23	2.03	0.40
2:D:1414:LYS:HZ3	2:D:1418:LYS:HD3	1.81	0.40
1:E:362:ASP:O	1:E:366:VAL:HG23	2.21	0.40
1:G:199:PRO:CG	1:G:200:GLU:N	2.85	0.40
1:G:308:ASN:OD1	1:G:313:LYS:O	2.40	0.40
1:A:506:ARG:HD2	1:A:506:ARG:N	2.37	0.40
2:B:1354:ARG:HA	2:B:1354:ARG:HD3	1.91	0.40
1:G:185:ARG:CG	1:G:185:ARG:NH1	2.81	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	440/598 (74%)	412 (94%)	22 (5%)	6 (1%)	11 20
1	C	435/598 (73%)	409 (94%)	18 (4%)	8 (2%)	8 14
1	E	435/598 (73%)	414 (95%)	16 (4%)	5 (1%)	14 26
1	G	430/598 (72%)	400 (93%)	19 (4%)	11 (3%)	5 8
2	B	171/180 (95%)	163 (95%)	7 (4%)	1 (1%)	25 43
2	D	176/180 (98%)	166 (94%)	8 (4%)	2 (1%)	14 26
2	F	174/180 (97%)	164 (94%)	7 (4%)	3 (2%)	9 16
2	H	177/180 (98%)	168 (95%)	8 (4%)	1 (1%)	25 43
All	All	2438/3112 (78%)	2296 (94%)	105 (4%)	37 (2%)	10 18

All (37) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	158	SER
1	A	517	ASP
1	A	585	GLU
1	C	157	PRO
1	C	199	PRO
1	C	517	ASP
1	C	585	GLU
1	E	517	ASP
1	E	585	GLU
2	F	1438	GLU
1	G	177	ALA
1	G	198	CYS
1	G	200	GLU
1	G	517	ASP
1	G	585	GLU
1	A	584	ALA
2	B	1300	GLY
1	C	153	PRO
1	C	197	GLY
1	C	200	GLU
1	C	584	ALA
2	D	1300	GLY
1	E	584	ALA
2	F	1300	GLY
1	G	584	ALA
2	H	1300	GLY
1	E	199	PRO
1	G	176	LEU
1	G	199	PRO
2	D	1437	ALA
2	F	1437	ALA
1	A	487	SER
1	G	167	ARG
1	G	581	ALA
1	A	490	GLY
1	E	167	ARG
1	G	158	SER

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	389/527 (74%)	361 (93%)	28 (7%)	14	28
1	C	389/527 (74%)	356 (92%)	33 (8%)	10	21
1	E	387/527 (73%)	350 (90%)	37 (10%)	8	16
1	G	385/527 (73%)	347 (90%)	38 (10%)	8	15
2	B	162/168 (96%)	147 (91%)	15 (9%)	9	17
2	D	167/168 (99%)	152 (91%)	15 (9%)	9	19
2	F	165/168 (98%)	149 (90%)	16 (10%)	8	16
2	H	168/168 (100%)	154 (92%)	14 (8%)	11	22
All	All	2212/2780 (80%)	2016 (91%)	196 (9%)	9	19

All (196) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	160	LYS
1	A	163	SER
1	A	173	SER
1	A	181	SER
1	A	185	ARG
1	A	190	ASN
1	A	191	ILE
1	A	209	MET
1	A	266	ASN
1	A	313	LYS
1	A	334	ASP
1	A	339	GLN
1	A	370	ASP
1	A	373	ASP
1	A	393	LEU
1	A	425	SER
1	A	428	ASP
1	A	429	VAL
1	A	447	ARG
1	A	448	GLU
1	A	480	LEU
1	A	506	ARG
1	A	515	GLN
1	A	518	MET

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Mol	Chain	Res	Type
1	A	561	ARG
1	A	582	ASP
1	A	586	ARG
1	A	587	GLN
2	B	1274	ARG
2	B	1301	THR
2	B	1308	TYR
2	B	1316	LYS
2	B	1347	ILE
2	B	1366	ARG
2	B	1376	LYS
2	B	1396	ARG
2	B	1406	GLU
2	B	1410	THR
2	B	1417	LEU
2	B	1418	LYS
2	B	1420	GLN
2	B	1428	GLN
2	B	1431	ARG
1	C	153	PRO
1	C	158	SER
1	C	159	GLN
1	C	164	ARG
1	C	166	ASN
1	C	178	GLN
1	C	185	ARG
1	C	190	ASN
1	C	196	LEU
1	C	199	PRO
1	C	202	LEU
1	C	243	LEU
1	C	268	LYS
1	C	279	SER
1	C	292	LYS
1	C	344	VAL
1	C	385	LYS
1	C	400	ASP
1	C	406	LEU
1	C	418	SER
1	C	425	SER
1	C	441	SER
1	C	443	SER

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Mol	Chain	Res	Type
1	C	447	ARG
1	C	448	GLU
1	C	507	SER
1	C	518	MET
1	C	524	SER
1	C	540	ILE
1	C	575	TYR
1	C	582	ASP
1	C	586	ARG
1	C	594	GLN
2	D	1268	THR
2	D	1270	GLU
2	D	1320	LEU
2	D	1332	MET
2	D	1335	ARG
2	D	1354	ARG
2	D	1357	THR
2	D	1376	LYS
2	D	1405	LEU
2	D	1408	LEU
2	D	1411	ASP
2	D	1416	LYS
2	D	1420	GLN
2	D	1440	PHE
2	D	1443	ARG
1	E	159	GLN
1	E	164	ARG
1	E	173	SER
1	E	190	ASN
1	E	198	CYS
1	E	199	PRO
1	E	203	THR
1	E	206	TYR
1	E	231	LEU
1	E	236	LYS
1	E	241	THR
1	E	248	GLN
1	E	291	LEU
1	E	307	ILE
1	E	308	ASN
1	E	336	ASP
1	E	361	LEU

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Mol	Chain	Res	Type
1	E	382	LEU
1	E	403	LYS
1	E	418	SER
1	E	425	SER
1	E	447	ARG
1	E	448	GLU
1	E	451	LYS
1	E	452	GLN
1	E	506	ARG
1	E	507	SER
1	E	518	MET
1	E	538	LEU
1	E	540	ILE
1	E	544	LEU
1	E	561	ARG
1	E	564	LYS
1	E	575	TYR
1	E	585	GLU
1	E	586	ARG
1	E	594	GLN
2	F	1301	THR
2	F	1309	ARG
2	F	1311	SER
2	F	1313	ILE
2	F	1321	THR
2	F	1332	MET
2	F	1340	LYS
2	F	1350	GLU
2	F	1366	ARG
2	F	1411	ASP
2	F	1412	HIS
2	F	1416	LYS
2	F	1420	GLN
2	F	1425	LYS
2	F	1440	PHE
2	F	1441	LEU
1	G	159	GLN
1	G	160	LYS
1	G	166	ASN
1	G	167	ARG
1	G	176	LEU
1	G	185	ARG

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Mol	Chain	Res	Type
1	G	190	ASN
1	G	199	PRO
1	G	207	LYS
1	G	209	MET
1	G	221	THR
1	G	236	LYS
1	G	249	GLU
1	G	265	LEU
1	G	271	ILE
1	G	276	ARG
1	G	292	LYS
1	G	312	ARG
1	G	321	GLU
1	G	329	GLN
1	G	332	GLU
1	G	336	ASP
1	G	340	SER
1	G	382	LEU
1	G	396	SER
1	G	425	SER
1	G	443	SER
1	G	452	GLN
1	G	506	ARG
1	G	515	GLN
1	G	518	MET
1	G	538	LEU
1	G	540	ILE
1	G	544	LEU
1	G	575	TYR
1	G	582	ASP
1	G	586	ARG
1	G	591	ILE
2	H	1266	GLN
2	H	1267	LEU
2	H	1274	ARG
2	H	1289	GLU
2	H	1302	ASP
2	H	1309	ARG
2	H	1315	CYS
2	H	1316	LYS
2	H	1320	LEU
2	H	1332	MET

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Mol	Chain	Res	Type
2	H	1362	LEU
2	H	1391	GLN
2	H	1415	ASP
2	H	1420	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (50) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	166	ASN
1	A	190	ASN
1	A	256	GLN
1	A	283	GLN
1	A	369	HIS
1	A	386	HIS
1	A	566	GLN
1	A	587	GLN
2	B	1294	ASN
1	C	166	ASN
1	C	178	GLN
1	C	248	GLN
1	C	256	GLN
1	C	283	GLN
1	C	369	HIS
1	C	386	HIS
1	C	515	GLN
2	D	1290	ASN
2	D	1294	ASN
2	D	1359	HIS
2	D	1439	GLN
1	E	190	ASN
1	E	256	GLN
1	E	283	GLN
1	E	308	ASN
1	E	329	GLN
1	E	369	HIS
1	E	386	HIS
1	E	419	HIS
1	E	452	GLN
1	E	566	GLN
2	F	1294	ASN
2	F	1363	GLN
2	F	1412	HIS

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Mol	Chain	Res	Type
1	G	190	ASN
1	G	256	GLN
1	G	283	GLN
1	G	329	GLN
1	G	339	GLN
1	G	369	HIS
1	G	386	HIS
1	G	391	ASN
1	G	452	GLN
1	G	515	GLN
1	G	566	GLN
2	H	1290	ASN
2	H	1294	ASN
2	H	1312	ASN
2	H	1420	GLN
2	H	1439	GLN

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)

Of 8 ligands modelled in this entry, 8 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	442/598 (73%)	-0.07	12 (2%)	54	58	18, 42, 87, 110	0
1	C	441/598 (73%)	-0.12	14 (3%)	47	51	16, 35, 86, 106	0
1	E	439/598 (73%)	-0.14	6 (1%)	75	77	20, 38, 86, 105	0
1	G	436/598 (72%)	0.03	9 (2%)	63	66	31, 53, 91, 115	0
2	B	173/180 (96%)	0.45	18 (10%)	6	6	15, 55, 104, 116	0
2	D	178/180 (98%)	0.22	14 (7%)	12	12	17, 50, 96, 110	0
2	F	176/180 (97%)	0.03	7 (3%)	38	41	26, 48, 89, 104	0
2	H	179/180 (99%)	0.89	36 (20%)	1	0	39, 71, 105, 118	0
All	All	2464/3112 (79%)	0.06	116 (4%)	31	33	15, 46, 94, 118	0

All (116) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	1300	GLY	8.4
1	C	152	SER	8.3
1	G	580	ALA	7.4
2	D	1300	GLY	6.5
2	H	1412	HIS	5.8
2	B	1299	SER	5.4
2	B	1410	THR	5.3
1	G	582	ASP	5.1
2	D	1408	LEU	5.0
2	F	1267	LEU	4.9
2	F	1266	GLN	4.9
2	H	1300	GLY	4.7
2	H	1407	LYS	4.6
2	H	1301	THR	4.6
2	B	1409	THR	4.5
2	H	1405	LEU	4.4

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Mol	Chain	Res	Type	RSRZ
2	D	1417	LEU	4.3
1	C	153	PRO	4.2
1	A	491	THR	4.2
2	H	1410	THR	4.2
2	H	1266	GLN	4.1
2	D	1409	THR	4.1
2	D	1299	SER	4.0
1	G	202	LEU	3.9
2	F	1313	ILE	3.9
2	H	1413	GLU	3.9
2	H	1409	THR	3.7
1	E	335	ALA	3.7
2	B	1417	LEU	3.7
1	A	332	GLU	3.7
1	A	585	GLU	3.6
2	H	1411	ASP	3.6
1	C	311	GLY	3.5
1	E	332	GLU	3.5
2	F	1412	HIS	3.4
2	H	1421	PHE	3.4
2	B	1440	PHE	3.3
2	H	1287	GLY	3.3
1	G	585	GLU	3.3
1	E	585	GLU	3.3
1	C	584	ALA	3.2
1	C	312	ARG	3.2
2	F	1440	PHE	3.2
2	B	1414	LYS	3.2
1	C	198	CYS	3.2
2	D	1413	GLU	3.1
2	D	1421	PHE	3.1
1	E	206	TYR	3.1
2	H	1440	PHE	3.1
2	H	1316	LYS	3.1
1	C	585	GLU	3.1
2	D	1301	THR	3.0
2	D	1405	LEU	3.0
2	B	1422	PHE	3.0
2	B	1411	ASP	3.0
2	B	1412	HIS	3.0
1	A	582	ASP	3.0
2	H	1267	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
2	B	1298	GLY	3.0
1	C	151	PHE	2.9
2	D	1412	HIS	2.9
2	F	1410	THR	2.8
2	D	1308	TYR	2.8
2	H	1415	ASP	2.8
2	D	1410	THR	2.7
2	B	1419	LYS	2.7
2	H	1308	TYR	2.7
1	A	489	SER	2.7
2	B	1301	THR	2.7
2	H	1441	LEU	2.7
2	H	1292	TYR	2.7
1	G	581	ALA	2.6
2	B	1415	ASP	2.6
1	A	187	GLY	2.6
2	H	1313	ILE	2.6
1	A	581	ALA	2.5
2	H	1268	THR	2.5
1	C	583	GLY	2.5
2	B	1303	MET	2.5
1	A	335	ALA	2.5
1	C	202	LEU	2.5
1	A	336	ASP	2.5
1	G	584	ALA	2.5
2	H	1422	PHE	2.4
2	H	1408	LEU	2.4
2	B	1311	SER	2.4
1	E	581	ALA	2.4
1	G	187	GLY	2.4
2	F	1439	GLN	2.3
2	H	1299	SER	2.3
2	H	1291	ILE	2.3
2	B	1421	PHE	2.3
1	E	336	ASP	2.3
2	H	1416	LYS	2.3
2	H	1314	ASP	2.3
1	A	393	LEU	2.2
2	H	1443	ARG	2.2
1	A	189	GLY	2.2
1	C	188	ALA	2.2
1	C	201	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
2	D	1407	LYS	2.2
2	H	1280	LYS	2.2
2	H	1269	ASP	2.2
2	H	1373	ALA	2.1
2	H	1304	GLU	2.1
2	H	1419	LYS	2.1
1	C	181	SER	2.1
1	C	447	ARG	2.1
2	B	1305	PRO	2.1
1	G	200	GLU	2.1
1	G	336	ASP	2.1
2	H	1444	SER	2.1
2	H	1303	MET	2.1
1	A	448	GLU	2.1
2	D	1298	GLY	2.1
2	H	1417	LEU	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	ZN	H	1501	1/1	0.93	0.05	88,88,88,88	0
3	ZN	F	1502	1/1	0.96	0.10	62,62,62,62	0
3	ZN	B	1501	1/1	0.96	0.04	82,82,82,82	0
3	ZN	H	1502	1/1	0.98	0.09	64,64,64,64	0
3	ZN	F	1501	1/1	0.99	0.07	53,53,53,53	0
3	ZN	D	1501	1/1	0.99	0.06	66,66,66,66	0
3	ZN	B	1502	1/1	1.00	0.14	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	ZN	D	1502	1/1	1.00	0.10	43,43,43,43	0

6.5 Other polymers (i)

There are no such residues in this entry.