



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 10:34 PM GMT

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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

---

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

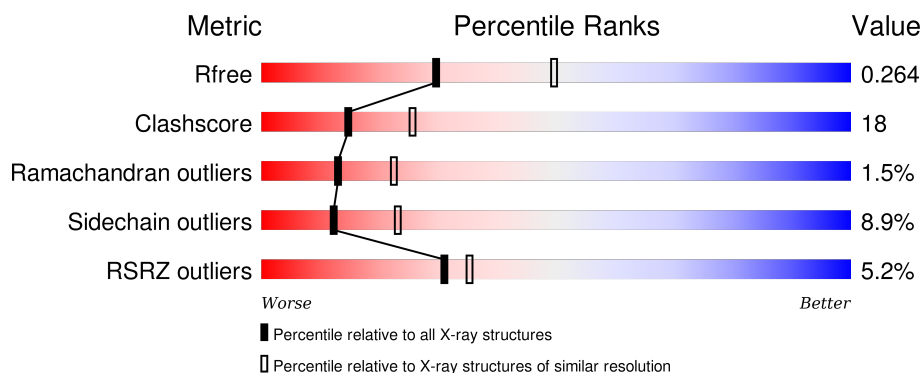
# 1 Overall quality at a glance

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))
$R_{free}$	91344	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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  $\leq 5\%$ . 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	<div> <div>2%</div> <div> <div></div> <div>50%</div> <div>21%</div> <div>•</div> <div>26%</div> </div> </div>
1	C	598	<div> <div>3%</div> <div> <div></div> <div>51%</div> <div>19%</div> <div>• •</div> <div>26%</div> </div> </div>
1	E	598	<div> <div>•</div> <div> <div></div> <div>53%</div> <div>17%</div> <div>•</div> <div>27%</div> </div> </div>
1	G	598	<div> <div>2%</div> <div> <div></div> <div>47%</div> <div>21%</div> <div>5%</div> <div>•</div> <div>27%</div> </div> </div>
2	B	180	<div> <div>11%</div> <div> <div></div> <div>56%</div> <div>35%</div> <div>6%</div> <div>•</div> </div> </div>

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
2	D	180	
2	F	180	
2	H	180	

## 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
1	A	442	Total	C	N	O	S	0	0	0
			3439	2187	574	663	15			
1	C	441	Total	C	N	O	S	0	0	0
			3435	2187	573	660	15			
1	E	439	Total	C	N	O	S	0	0	0
			3422	2178	571	658	15			
1	G	436	Total	C	N	O	S	0	0	0
			3400	2164	568	653	15			

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

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

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

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

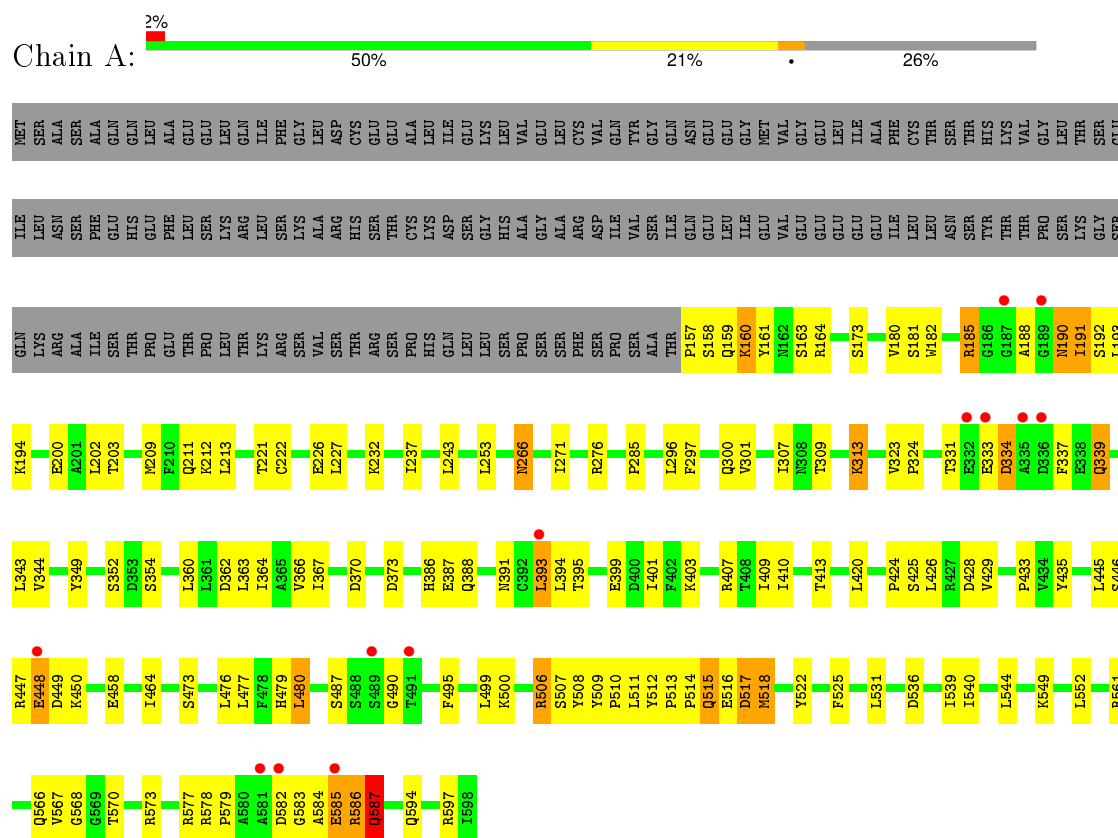
- Molecule 4 is water.

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

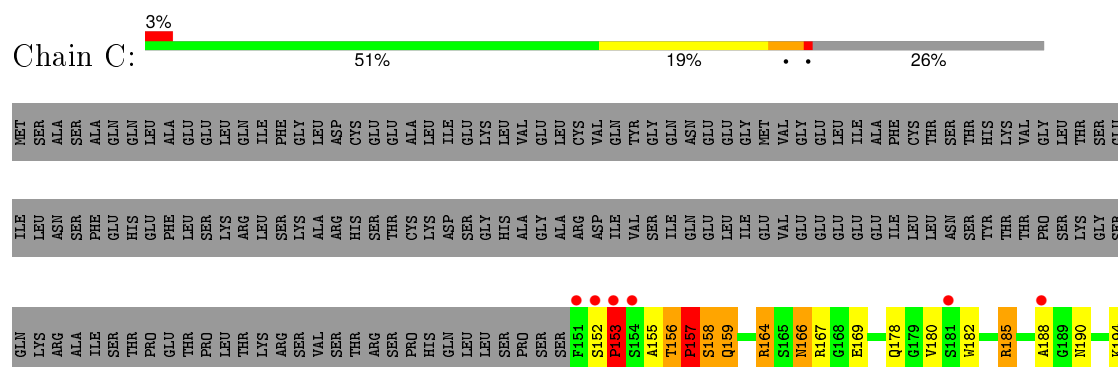
### 3 Residue-property plots

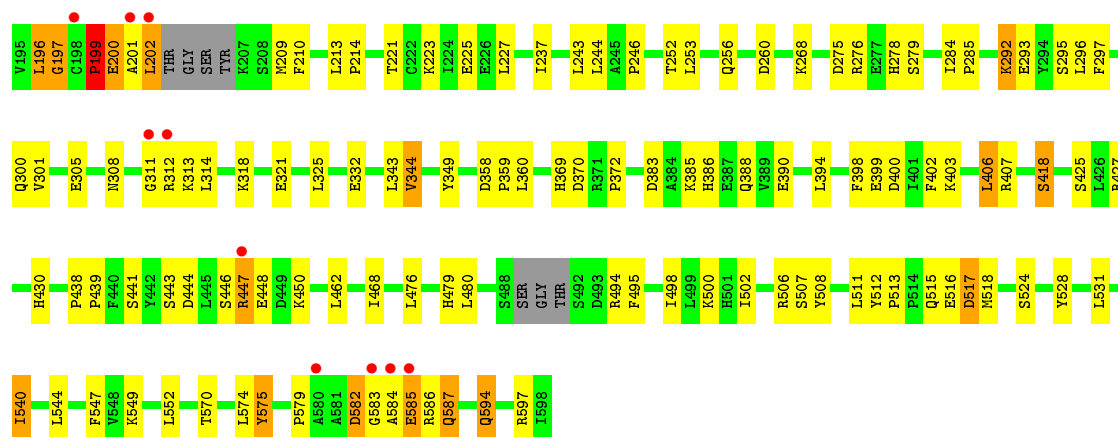
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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

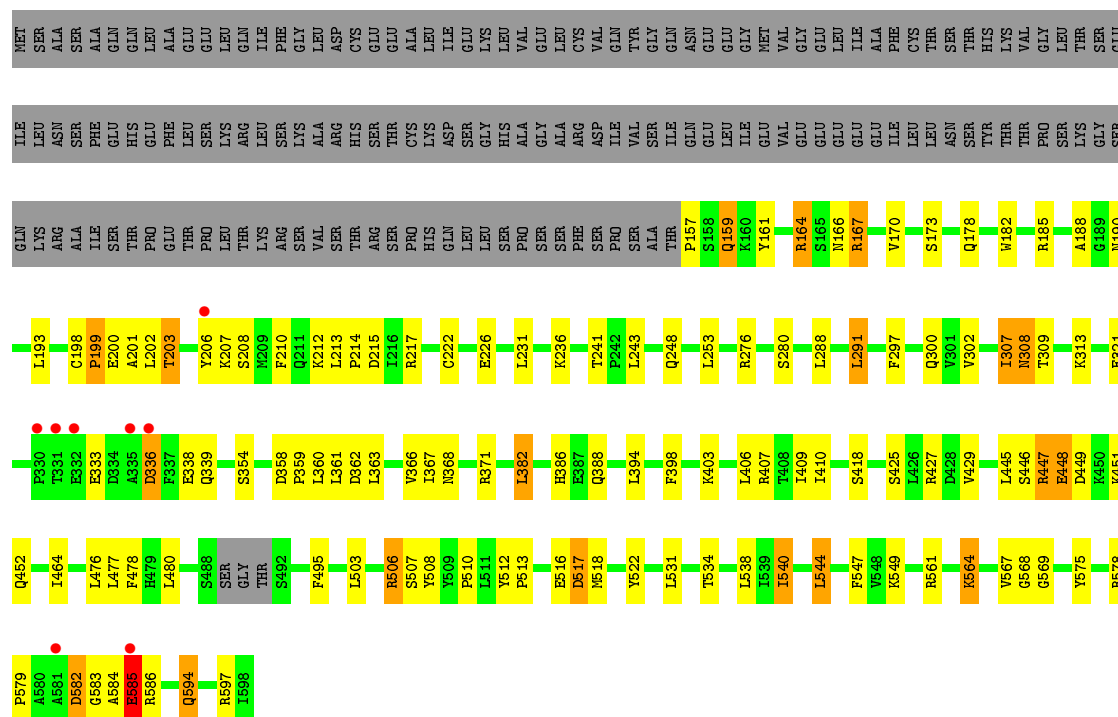


#### • Molecule 1: DNA polymerase alpha subunit B

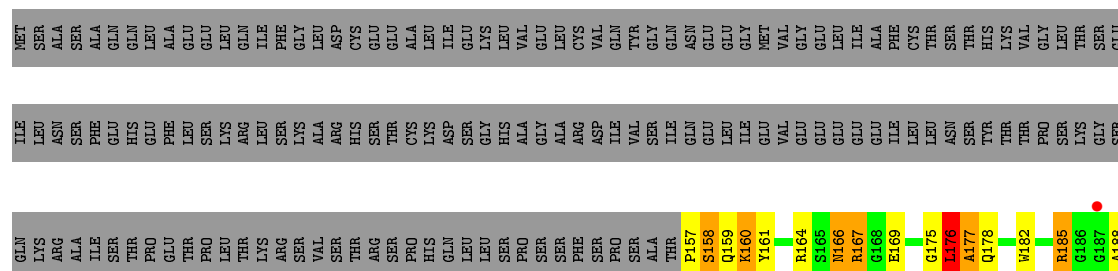


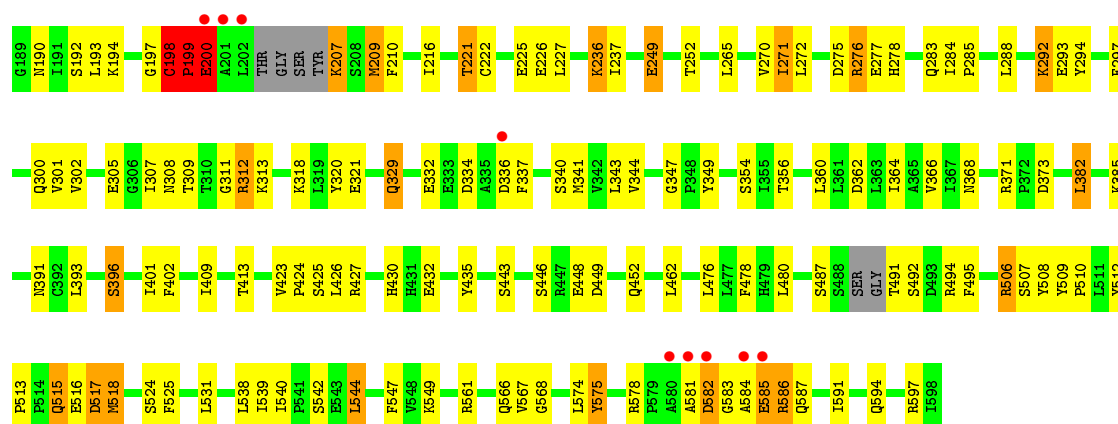


• Molecule 1: DNA polymerase alpha subunit B

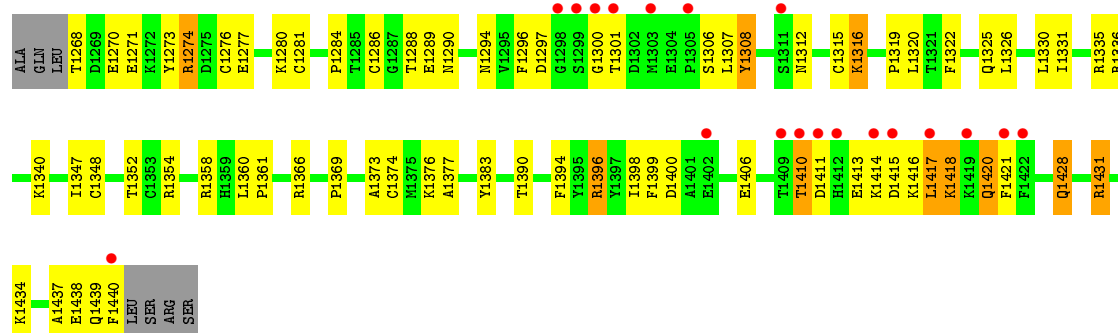


• Molecule 1: DNA polymerase alpha subunit B

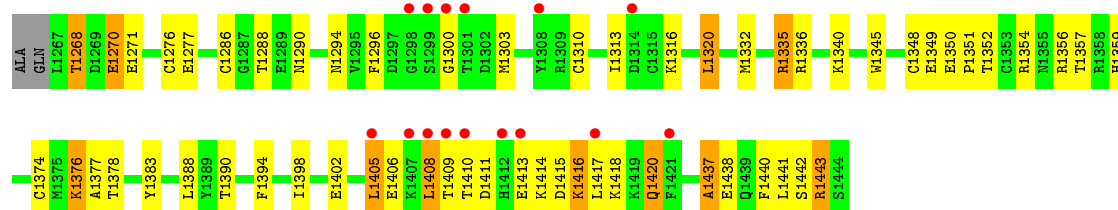




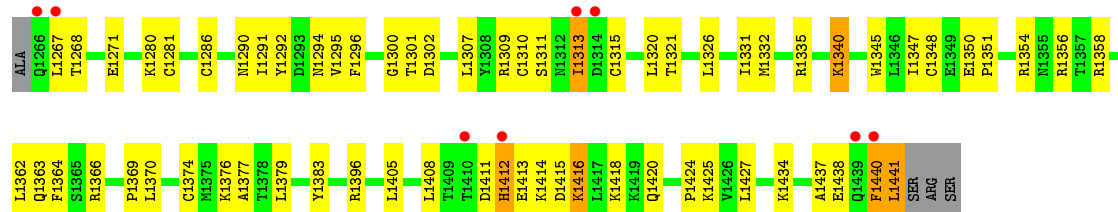
• Molecule 2: DNA polymerase alpha catalytic subunit



• Molecule 2: DNA polymerase alpha catalytic subunit

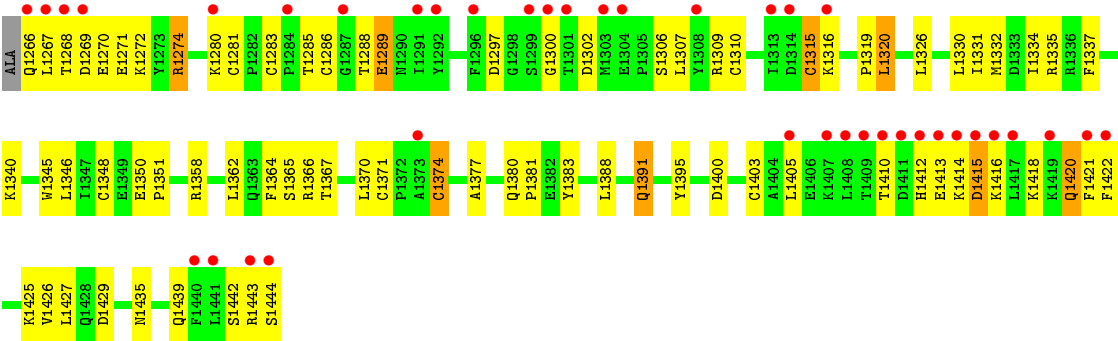


• Molecule 2: DNA polymerase alpha catalytic subunit



• Molecule 2: DNA polymerase alpha catalytic subunit





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	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	5892 reflections (5.04%)	DCC
Wilson B-factor (Å <sup>2</sup> )	31.2	Xtriage
Anisotropy	0.639	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 53.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 116887 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	19724	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

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(°)	Ideal(°)
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

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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 ⓘ

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

*Continued on next page...*

*Continued from previous page...*

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:HB3	1:C:185:ARG:HH11	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:HH11	1:E:164:ARG:HG3	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:H	2:F:1313:ILE:HD13	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:HA	2:D:1376:LYS:HE2	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

*Continued on next page...*

*Continued from previous page...*

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:HH11	1:A:506:ARG:HG2	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:HD22	1:C:166:ASN:H	0.81	0.79
1:C:185:ARG:HB2	1:C:188:ALA:HB3	1.63	0.79
2:B:1414:LYS:HG3	2:B:1415:ASP:N	1.96	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:HD3	1:G:292:LYS:H	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
2:H:1410:THR:HG22	2:H:1412:HIS:H	1.51	0.76
1:E:516:GLU:O	1:E:517:ASP:HB2	1.86	0.76
2:D:1414:LYS:NZ	2:D:1418:LYS:HD3	2.00	0.75
1:C:407:ARG:HH11	1:C:407:ARG:HG3	1.51	0.75
1:G:516:GLU:O	1:G:517:ASP:HB2	1.84	0.75
1:G:209:MET:HG2	1:G:209:MET:O	1.86	0.75
1:E:386:HIS:HD2	1:E:388:GLN:H	1.34	0.75
1:A:160:LYS:H	1:A:160:LYS:CD	2.00	0.73
2:F:1313:ILE:N	2:F:1313:ILE:HD13	2.03	0.73
2:D:1402:GLU:O	2:D:1406:GLU:HG2	1.86	0.73
1:A:271:ILE:C	1:A:271:ILE:HD12	2.08	0.73
1:A:313:LYS:HB2	1:A:313:LYS:NZ	2.03	0.73

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:1307:LEU:HD11	2:B:1326:LEU:HD11	1.71	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:H:1307:LEU:HD11	2:H:1326:LEU:HD11	1.72	0.71
1:C:152:SER:HB3	1:C:153:PRO:CD	2.19	0.71
2:B:1360:LEU:HD12	2:B:1361:PRO:HD2	1.71	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:HH11	1:G:506:ARG:HG2	1.56	0.70
1:G:185:ARG:HG2	1:G:188:ALA:HB3	1.73	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
2:F:1416:LYS:HB3	2:F:1416:LYS:NZ	2.07	0.69
2:F:1294:ASN:HD22	2:F:1296:PHE:H	1.38	0.69
2:H:1268:THR:HB	2:H:1271:GLU:OE1	1.92	0.69
2:B:1268:THR:HB	2:B:1271:GLU:CG	2.23	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:HA	1:C:332:GLU:OE2	1.94	0.68
2:F:1280:LYS:HG2	2:F:1291:ILE:HG12	1.76	0.68
1:C:292:LYS:H	1:C:292:LYS:HD2	1.58	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
2:D:1376:LYS:O	2:D:1376:LYS:HD3	1.95	0.67
1:C:196:LEU:HD23	1:C:197:GLY:H	1.58	0.67

*Continued on next page...*

*Continued from previous page...*

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
2:F:1294:ASN:ND2	2:F:1296:PHE:H	1.93	0.66
1:C:196:LEU:CD2	1:C:197:GLY:H	2.08	0.66
1:C:403:LYS:NZ	1:E:407:ARG:HH22	1.94	0.66
1:C:275:ASP:OD2	1:C:278:HIS:ND1	2.26	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:A:185:ARG:HB3	1:A:188:ALA:HB3	1.78	0.66
1:G:175:GLY:O	1:G:177:ALA:N	2.29	0.66
2:F:1268:THR:CG2	2:F:1271:GLU:HG2	2.24	0.66
1:A:388:GLN:HB3	1:A:393:LEU:CD2	2.26	0.66
1:E:477:LEU:HD11	1:E:540:ILE:HD13	1.78	0.65
1:G:207:LYS:HE2	1:G:524:SER:OG	1.97	0.65
1:C:194:LYS:HE3	4:C:618:HOH:O	1.96	0.65
2:B:1417:LEU:HD13	2:B:1421:PHE:CD1	2.30	0.65
2:B:1331:ILE:HG23	2:B:1440:PHE:HZ	1.60	0.65
1:G:185:ARG:HG3	1:G:185:ARG:HH11	1.61	0.65
1:C:292:LYS:N	1:C:292:LYS:HD2	2.11	0.65
1:G:164:ARG:HG2	1:G:164:ARG:HH11	1.61	0.65
1:E:446:SER:HB2	1:E:448:GLU:HG2	1.77	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:NH1	1:A:506:ARG:HG2	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
2:D:1313:ILE:N	2:D:1313:ILE:HD12	2.10	0.64
1:A:386:HIS:CD2	1:A:388:GLN:H	2.16	0.64
2:F:1412:HIS:CD2	2:F:1413:GLU:H	2.16	0.64
2:H:1391:GLN:HE21	2:H:1391:GLN:CA	2.11	0.64
1:C:480:LEU:HD23	1:C:498:ILE:HG23	1.80	0.64
1:G:432:GLU:HG3	2:H:1442:SER:CB	2.28	0.63

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:386:HIS:HD2	1:C:388:GLN:H	1.46	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
2:H:1307:LEU:HD11	2:H:1326:LEU:CD1	2.29	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
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
1:C:156:THR:CG2	1:C:159:GLN:HB3	2.29	0.62
2:B:1331:ILE:HG23	2:B:1440:PHE:CZ	2.35	0.62
1:C:221:THR:HG21	1:C:276:ARG:HB3	1.81	0.62
1:G:506:ARG:NH1	1:G:506:ARG:HG2	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:HH11	1:G:586:ARG:HG3	1.63	0.62
1:A:313:LYS:HB2	1:A:313:LYS:HZ3	1.63	0.61
1:C:308:ASN:ND2	1:C:311:GLY:HA2	2.15	0.61
1:A:476:LEU:HD11	1:A:510:PRO:HD2	1.82	0.61
1:G:185:ARG:HG3	1:G:188:ALA:HB3	1.81	0.61
1:C:157:PRO:O	1:C:158:SER:HB2	1.98	0.61
1:G:275:ASP:OD2	1:G:278:HIS:ND1	2.29	0.61
1:A:587:GLN:HA	1:A:587:GLN:HE21	1.64	0.61
2:F:1348:CYS:SG	2:F:1377:ALA:HB3	2.41	0.61
1:C:407:ARG:NH1	1:C:407:ARG:HG3	2.15	0.61
2:H:1340:LYS:HG2	2:H:1383:TYR:CD2	2.36	0.61
1:C:209:MET:HA	2:D:1443:ARG:HG3	1.82	0.61
2:B:1316:LYS:O	2:B:1316:LYS:HE3	2.00	0.61
1:G:292:LYS:CD	1:G:292:LYS:H	2.07	0.61
2:F:1307:LEU:HB3	2:F:1320:LEU:CD2	2.31	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:C:209:MET:HA	2:D:1443:ARG:CG	2.32	0.60
1:A:424:PRO:O	1:A:458:GLU:HG3	2.01	0.60

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:1412:HIS:CD2	2:F:1413:GLU:N	2.69	0.60
2:F:1340:LYS:HD2	2:F:1383:TYR:CD2	2.37	0.60
1:A:394:LEU:HD13	1:A:401:ILE:CD1	2.32	0.59
1:G:586:ARG:NH1	1:G:586:ARG:HG3	2.17	0.59
1:C:312:ARG:HH11	1:C:313:LYS:HB3	1.66	0.59
1:A:500:LYS:HE3	1:A:552:LEU:HD21	1.83	0.59
1:E:164:ARG:HE	1:E:167:ARG:NH2	2.00	0.59
1:G:209:MET:CB	2:H:1443:ARG:HB3	2.20	0.59
1:E:308:ASN:ND2	1:E:313:LYS:O	2.34	0.59
1:A:182:TRP:CE3	1:A:573:ARG:HD3	2.37	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:HB2	1.84	0.59
1:C:500:LYS:HE3	1:C:552:LEU:HD21	1.85	0.59
2:H:1414:LYS:CG	2:H:1415:ASP:N	2.65	0.59
1:C:156:THR:HG23	1:C:159:GLN:HB3	1.83	0.59
1:G:311:GLY:O	1:G:312:ARG:HD2	2.02	0.59
1:C:200:GLU:HG2	1:C:528:TYR:CD1	2.38	0.59
1:G:164:ARG:NH1	1:G:164:ARG:HG2	2.18	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
1:E:386:HIS:CD2	1:E:388:GLN:H	2.18	0.58
2:B:1277:GLU:OE2	2:B:1336:ARG:NH2	2.37	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
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
2:B:1340:LYS:HD3	2:B:1383:TYR:CG	2.39	0.57
1:G:334:ASP:HA	1:G:337:PHE:CE2	2.38	0.57
1:G:271:ILE:HD13	1:G:283:GLN:HB3	1.85	0.57
1:A:243:LEU:HD22	1:A:253:LEU:HD13	1.87	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

*Continued on next page...*

*Continued from previous page...*

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:NE	1:C:447:ARG:O	2.38	0.56
1:C:292:LYS:HG2	1:C:293:GLU:N	2.20	0.56
1:C:292:LYS:CD	1:C:292:LYS:H	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
1:E:157:PRO:HB3	1:E:354:SER:HB3	1.87	0.56
2:D:1340:LYS:HD3	2:D:1383:TYR:CD2	2.41	0.56
1:G:308:ASN:ND2	1:G:311:GLY:HA2	2.21	0.56
1:A:579:PRO:HG3	1:A:587:GLN:HB3	1.88	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
2:H:1350:GLU:OE2	2:H:1351:PRO:HD2	2.05	0.55
1:E:338:GLU:HG2	1:E:339:GLN:N	2.21	0.55
1:C:343:LEU:HD23	1:C:344:VAL:N	2.21	0.55
1:A:448:GLU:OE1	1:A:448:GLU:HA	2.06	0.55
1:G:426:LEU:HD21	1:G:435:TYR:HB2	1.88	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: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:313:LYS:CE	2:F:1313:ILE:HB	2.36	0.55
1:A:160:LYS:N	1:A:160:LYS:CD	2.70	0.55
1:E:495:PHE:HB2	1:E:549:LYS:HE3	1.89	0.55
1:G:297:PHE:CE1	1:G:300:GLN:HB2	2.42	0.54
2:B:1281:CYS:SG	2:B:1326:LEU:HD23	2.47	0.54
2:H:1330:LEU:O	2:H:1334:ILE:HG13	2.06	0.54
1:G:157:PRO:O	1:G:158:SER:HB2	2.05	0.54
1:G:185:ARG:CD	1:G:373:ASP:OD2	2.55	0.54
1:G:160:LYS:HZ2	1:G:566:GLN:HE21	1.55	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: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
1:A:344:VAL:HG11	1:A:539:ILE:HG21	1.90	0.54

*Continued on next page...*

*Continued from previous page...*

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:G:341:MET:HG3	1:G:575:TYR:CE1	2.42	0.54
1:C:325:LEU:HD21	1:C:506:ARG:HD3	1.90	0.54
2:D:1409:THR:HG23	2:D:1410:THR:H	1.71	0.54
2:B:1331:ILE:O	2:B:1335:ARG:HG3	2.07	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:445:LEU:HD22	1:A:449:ASP:HB3	1.90	0.54
1:A:202:LEU:HD23	1:A:202:LEU:C	2.28	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:1413:GLU:HA	2:H:1416:LYS:CE	2.37	0.53
2:H:1337:PHE:HE2	2:H:1395:TYR:CE2	2.26	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:G:275:ASP:CG	1:G:278:HIS:HD1	2.12	0.53
2:F:1281:CYS:SG	2:F:1326:LEU:HD23	2.49	0.53
1:C:180:VAL:O	1:C:180:VAL:HG12	2.09	0.53
1:C:213:LEU:HB2	1:C:214:PRO:HD3	1.91	0.53
1:G:199:PRO:CG	1:G:200:GLU:H	2.19	0.53
1:C:221:THR:HG22	1:C:225:GLU:OE2	2.09	0.53
1:A:182:TRP:CD2	1:A:573:ARG:HD3	2.43	0.53
2:B:1438:GLU:N	2:B:1438:GLU:OE1	2.42	0.53
2:B:1308:TYR:C	2:B:1308:TYR:CD1	2.82	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
2:F:1415:ASP:HA	2:F:1418:LYS:HB3	1.89	0.52
1:C:201:ALA:HA	1:C:439:PRO:CD	2.39	0.52
1:G:300:GLN:HG2	1:G:302:VAL:CG1	2.38	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:586:ARG:CG	1:G:586:ARG:HH11	2.23	0.52
1:C:182:TRP:HE1	1:C:594:GLN:HE22	1.58	0.52
1:G:209:MET:HE2	2:H:1444:SER:HB2	1.92	0.52
2:B:1410:THR:HG23	2:B:1413:GLU:HB3	1.92	0.52
2:D:1376:LYS:HE2	2:D:1376:LYS:CA	2.33	0.52
2:F:1307:LEU:HD23	2:F:1320:LEU:HD23	1.92	0.52

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:294:TYR:CD1	1:G:487:SER:HB3	2.44	0.52
1:C:295:SER:O	1:C:296:LEU:HD23	2.09	0.52
1:C:196:LEU:CD1	1:C:468:ILE:HD12	2.39	0.52
1:A:285:PRO:HG2	1:A:313:LYS:NZ	2.25	0.52
1:A:222:CYS:O	1:A:226:GLU:HB2	2.09	0.52
2:B:1307:LEU:HD11	2:B:1326:LEU:CD1	2.37	0.51
2:D:1416:LYS:HD2	2:D:1416:LYS:C	2.31	0.51
2:B:1276:CYS:SG	2:B:1390:THR:HG22	2.49	0.51
1:A:570:THR:HG22	1:A:597:ARG:HA	1.92	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
2:H:1413:GLU:CA	2:H:1416:LYS:HE3	2.41	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
1:A:192:SER:OG	1:A:194:LYS:HE3	2.09	0.51
1:G:207:LYS:HB2	1:G:207:LYS:HZ3	1.75	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:574:LEU:HD12	1:G:574:LEU:N	2.25	0.51
1:A:393:LEU:C	1:A:393:LEU:HD23	2.30	0.51
1:A:509:TYR:CE2	1:A:518:MET:SD	3.04	0.51
1:E:447:ARG:HH11	1:E:447:ARG:HB3	1.75	0.51
2:B:1330:LEU:HD11	2:B:1399:PHE:CE2	2.46	0.51
1:G:160:LYS:NZ	1:G:566:GLN:HE21	2.09	0.51
2:H:1391:GLN:C	2:H:1391:GLN:HE21	2.13	0.51
1:A:362:ASP:O	1:A:366:VAL:HG23	2.11	0.51
1:G:494:ARG:NH1	1:G:494:ARG:HG3	2.25	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:510:PRO:HA	4:G:607:HOH:O	2.11	0.51
1:G:307:ILE:HG23	1:G:309:THR:HG23	1.93	0.51
1:A:339:GLN:HG2	1:A:577:ARG:CZ	2.41	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:C:402:PHE:CD1	1:C:430:HIS:CE1	2.99	0.50
2:B:1270:GLU:CD	2:B:1270:GLU:C	2.69	0.50
1:G:271:ILE:HD12	1:G:271:ILE:C	2.32	0.50
1:A:360:LEU:HD11	1:A:409:ILE:HD11	1.93	0.50
1:E:583:GLY:O	1:E:585:GLU:N	2.45	0.50
1:E:202:LEU:HD12	2:H:1364:PHE:HB3	1.92	0.50
1:G:368:ASN:O	1:G:371:ARG:HG2	2.11	0.50

*Continued on next page...*

*Continued from previous page...*

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

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:308:ASN:HD21	1:G:311:GLY:HA2	1.78	0.49
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:385:LYS:HE2	1:G:427:ARG:HD2	1.94	0.49
2:B:1437:ALA:HB3	2:B:1438:GLU:OE1	2.13	0.48
1:A:213:LEU:HG	4:A:627:HOH:O	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:285:PRO:HD2	1:C:312:ARG:O	2.13	0.48
1:C:275:ASP:CG	1:C:278:HIS:HD1	2.15	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
2:F:1416:LYS:HB3	2:F:1416:LYS:HZ2	1.78	0.48
1:C:201:ALA:HA	1:C:439:PRO:HD3	1.94	0.48
1:A:586:ARG:HG3	1:A:586:ARG:HH11	1.77	0.48
2:H:1413:GLU:N	2:H:1416:LYS:HE3	2.28	0.48
2:D:1416:LYS:HG3	2:D:1417:LEU:N	2.27	0.48
1:C:152:SER:CB	1:C:153:PRO:CD	2.87	0.48
1:G:236:LYS:N	1:G:236:LYS:HD3	2.28	0.48
2:H:1412:HIS:O	2:H:1416:LYS:CG	2.51	0.48
1:G:221:THR:HG22	1:G:225:GLU:OE2	2.13	0.48
2:B:1308:TYR:C	2:B:1308:TYR:HD1	2.17	0.48
2:F:1268:THR:HG22	2:F:1271:GLU:CD	2.34	0.48
1:A:227:LEU:HD23	1:A:301:VAL:CB	2.37	0.48
1:G:311:GLY:C	1:G:312:ARG:HD2	2.34	0.48
1:E:447:ARG:HG2	1:E:448:GLU:N	2.28	0.48
1:E:360:LEU:HD11	1:E:409:ILE:HD11	1.96	0.48
2:B:1352:THR:HG22	2:B:1352:THR:O	2.14	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:E:164:ARG:NE	1:E:167:ARG:NH2	2.62	0.47
1:A:297:PHE:CG	1:A:480:LEU:HD11	2.49	0.47
1:E:321:GLU:HB2	4:E:635:HOH:O	2.12	0.47
1:A:583:GLY:O	1:A:585:GLU:N	2.47	0.47
1:C:152:SER:CB	1:C:153:PRO:HD2	2.29	0.47
1:C:313:LYS:HG2	1:C:314:LEU:N	2.29	0.47
1:C:199:PRO:O	1:C:200:GLU:HB2	2.14	0.47
1:E:243:LEU:HD22	1:E:253:LEU:HD13	1.96	0.47
2:H:1420:GLN:HE21	2:H:1420:GLN:C	2.17	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:512:TYR:HA	1:E:513:PRO:C	2.33	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:E:164:ARG:CG	1:E:164:ARG:NH1	2.67	0.47
1:C:402:PHE:CE2	1:C:406:LEU:HD22	2.49	0.47
1:A:512:TYR:HA	1:A:513:PRO:C	2.35	0.47
1:A:426:LEU:HD11	1:A:435:TYR:HB2	1.96	0.47
1:A:333:GLU:H	1:A:333:GLU:CD	2.17	0.47
2:B:1348:CYS:SG	2:B:1377:ALA:HB3	2.55	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:HA	1:G:382:LEU:HD23	1.72	0.47
1:C:221:THR:CG2	1:C:276:ARG:H	2.28	0.47
2:B:1428:GLN:HG2	2:B:1431:ARG:HH21	1.80	0.47
1:G:271:ILE:HD12	1:G:272:LEU:C	2.35	0.47
2:F:1408:LEU:O	2:F:1414:LYS:HE3	2.15	0.47
1:E:157:PRO:N	1:E:159:GLN:OE1	2.48	0.46
1:G:237:ILE:HD11	1:G:320:TYR:CZ	2.50	0.46
1:A:363:LEU:O	1:A:367:ILE:HG13	2.15	0.46
1:A:266:ASN:HD22	2:F:1302:ASP:HA	1.80	0.46
1:E:445:LEU:HD22	1:E:449:ASP:HB3	1.95	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: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: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:A:307:ILE:HG23	1:A:309:THR:HG23	1.97	0.46
1:G:362:ASP:O	1:G:366:VAL:HG23	2.16	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:A:586:ARG:HH11	1:A:586:ARG:CG	2.29	0.46
2:F:1416:LYS:HB3	2:F:1416:LYS:HZ3	1.81	0.46
1:E:297:PHE:CG	1:E:480:LEU:HD11	2.50	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
2:H:1405:LEU:HD11	2:H:1422:PHE:CD2	2.51	0.46
2:H:1271:GLU:HG2	2:H:1274:ARG:NH2	2.25	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:F:1335:ARG:NH2	4:F:1607:HOH:O	2.49	0.46

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1349:GLU:O	2:D:1351:PRO:HD3	2.16	0.46
1:C:305:GLU:HB3	1:C:318:LYS:HB3	1.97	0.46
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
1:A:232:LYS:HG3	1:A:237:ILE:HB	1.98	0.45
2:B:1307:LEU:HD23	2:B:1320:LEU:CD2	2.46	0.45
1:E:476:LEU:HD22	1:E:508:TYR:O	2.16	0.45
1:E:445:LEU:CD2	1:E:449:ASP:HB3	2.46	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
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
2:D:1359:HIS:CD2	2:D:1359:HIS:C	2.90	0.45
1:A:446:SER:O	1:A:450:LYS:CG	2.63	0.45
1:G:182:TRP:HE1	1:G:594:GLN:NE2	2.15	0.45
1:E:213:LEU:HB2	1:E:214:PRO:HD3	1.99	0.45
2:H:1365:SER:HB3	2:H:1370:LEU:HD13	1.98	0.45
1:E:166:ASN:HB3	1:E:597:ARG:HD2	1.98	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:C:196:LEU:O	1:C:197:GLY:O	2.35	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:E:406:LEU:O	1:E:410:ILE:HG13	2.16	0.45
2:D:1348:CYS:SG	2:D:1377:ALA:HB3	2.56	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
2:H:1410:THR:HG22	2:H:1412:HIS:HB2	1.98	0.45
1:E:280:SER:O	2:F:1363:GLN:HG3	2.16	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: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
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:C:166:ASN:HB2	1:C:597:ARG:CD	2.47	0.44
1:A:160:LYS:HD3	1:A:160:LYS:H	1.78	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:156:THR:N	1:C:157:PRO:HD2	2.31	0.44
1:E:333:GLU:O	1:E:336:ASP:HB2	2.17	0.44
1:G:515:GLN:HB3	1:G:515:GLN:HE21	1.59	0.44
1:A:476:LEU:HD22	1:A:508:TYR:O	2.17	0.44
2:H:1283:CYS:SG	2:H:1285:THR:OG1	2.75	0.44
2:F:1440:PHE:HA	2:F:1440:PHE:HD1	1.66	0.44
1:G:547:PHE:C	1:G:547:PHE:CD1	2.91	0.44
1:G:222:CYS:O	1:G:226:GLU:HB2	2.17	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:G:508:TYR:CE2	1:G:531:LEU:HD23	2.53	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
2:B:1396:ARG:NH1	2:B:1434:LYS:HE2	2.32	0.44
2:H:1425:LYS:HD3	2:H:1429:ASP:OD2	2.17	0.44
2:H:1348:CYS:SG	2:H:1377:ALA:HB3	2.57	0.44
1:A:399:GLU:OE2	1:A:403:LYS:HE2	2.17	0.44
1:C:403:LYS:NZ	1:E:407:ARG:NH2	2.62	0.44
1:C:223:LYS:HZ1	1:C:256:GLN:HE21	1.65	0.44
2:F:1369:PRO:HG2	2:F:1379:LEU:HB2	1.99	0.44
1:A:212:LYS:HA	1:A:212:LYS:HD2	1.88	0.44
2:H:1380:GLN:OE1	2:H:1380:GLN:HA	2.18	0.44
1:G:297:PHE:CG	1:G:480:LEU:HD11	2.53	0.44
1:C:312:ARG:HD2	1:C:313:LYS:HB3	2.00	0.44
1:G:160:LYS:HZ1	1:G:566:GLN:NE2	2.14	0.44
1:C:547:PHE:CD1	1:C:547:PHE:C	2.91	0.44
2:H:1280:LYS:HD3	2:H:1289:GLU:OE1	2.17	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:D:1316:LYS:HE2	2:D:1316:LYS:HB3	1.82	0.44
1:C:383:ASP:OD2	1:C:427:ARG:NH2	2.37	0.44
1:C:202:LEU:HD23	1:C:202:LEU:O	2.17	0.44
2:H:1286:CYS:SG	2:H:1288:THR:HG23	2.58	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
1:G:176:LEU:HG	1:G:176:LEU:O	2.17	0.43
1:E:159:GLN:HG2	1:E:159:GLN:H	1.46	0.43
1:A:509:TYR:CE1	1:A:511:LEU:HB3	2.53	0.43
2:B:1417:LEU:HD13	2:B:1421:PHE:HD1	1.78	0.43
1:C:494:ARG:HG3	1:C:494:ARG:HH11	1.83	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:1362:LEU:N	2:F:1362:LEU:CD1	2.81	0.43
1:A:180:VAL:O	1:A:180:VAL:HG23	2.17	0.43
2:H:1422:PHE:HB3	2:H:1427:LEU:HD21	1.99	0.43
2:H:1320:LEU:HD12	2:H:1320:LEU:O	2.17	0.43
1:A:445:LEU:HD22	1:A:449:ASP:CB	2.47	0.43
1:A:193:LEU:CD2	1:A:464:ILE:HG12	2.48	0.43
1:A:507:SER:HG	1:A:525:PHE:HZ	1.65	0.43
1:E:200:GLU:OE2	1:E:203:THR:HG22	2.18	0.43
1:E:193:LEU:HD22	1:E:464:ILE:HG12	2.00	0.43
1:C:166:ASN:HB2	1:C:597:ARG:HD3	2.01	0.43
1:C:260:ASP:C	1:C:260:ASP:OD1	2.57	0.43
2:H:1391:GLN:NE2	2:H:1391:GLN:CA	2.81	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:F:1313:ILE:H	2:F:1313:ILE:CD1	2.01	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
1:A:221:THR:HG21	1:A:276:ARG:HB3	1.99	0.43
1:G:292:LYS:CD	1:G:292:LYS:N	2.72	0.43
1:A:271:ILE:O	1:A:271:ILE:HD12	2.18	0.43
1:A:413:THR:HG21	1:A:420:LEU:HD11	2.01	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
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
1:G:227:LEU:HD23	1:G:301:VAL:HB	2.01	0.43
2:D:1394:PHE:O	2:D:1398:ILE:HG23	2.19	0.43
1:C:574:LEU:HD12	1:C:574:LEU:N	2.33	0.43
1:C:210:PHE:HE1	2:D:1388:LEU:HD23	1.83	0.43
2:B:1268:THR:CG2	2:B:1271:GLU:HG2	2.50	0.42
1:G:586:ARG:HA	1:G:586:ARG:HD2	1.31	0.42
2:D:1276:CYS:SG	2:D:1390:THR:HG22	2.58	0.42
1:C:394:LEU:HD12	1:C:398:PHE:HE1	1.83	0.42
1:G:176:LEU:O	1:G:177:ALA:O	2.38	0.42
1:A:578:ARG:HA	1:A:579:PRO:HD2	1.87	0.42
1:E:201:ALA:HB3	2:H:1367:THR:C	2.39	0.42
2:B:1284:PRO:HG2	2:B:1322:PHE:CG	2.54	0.42
1:G:402:PHE:CD1	1:G:430:HIS:CE1	3.07	0.42
1:A:190:ASN:HD22	1:A:190:ASN:HA	1.56	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

*Continued on next page...*

*Continued from previous page...*

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

*Continued on next page...*

*Continued from previous page...*

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
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
2:D:1438:GLU:OE2	2:D:1441:LEU:HD12	2.20	0.41
1:A:386:HIS:HD2	1:A:388:GLN:N	2.12	0.41
2:H:1415:ASP:HA	2:H:1418:LYS:HB3	2.02	0.41
1:E:300:GLN:NE2	1:E:302:VAL:HG12	2.35	0.41
1:E:288:LEU:HD22	1:E:291:LEU:HD12	2.02	0.41
1:C:200:GLU:OE1	1:C:438:PRO:HA	2.20	0.41
1:A:182:TRP:CD2	1:A:573:ARG:CD	3.03	0.41
2:H:1345:TRP:CZ3	2:H:1358:ARG:HG3	2.56	0.41
1:A:323:VAL:HA	1:A:324:PRO:HD3	1.87	0.41
1:G:166:ASN:HB2	1:G:597:ARG:HD3	2.03	0.41
1:A:271:ILE:C	1:A:271:ILE:CD1	2.80	0.41
2:F:1396:ARG:HH12	2:F:1434:LYS:HE2	1.84	0.41
2:F:1354:ARG:HG2	2:F:1354:ARG:HH11	1.86	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:A:426:LEU:HD22	1:A:433:PRO:O	2.21	0.41
1:A:331:THR:OG1	1:A:334:ASP:OD1	2.38	0.41
1:A:331:THR:CB	1:A:333:GLU:OE2	2.69	0.41
1:E:578:ARG:HA	1:E:579:PRO:HD3	1.85	0.41
1:A:352:SER:H	1:A:352:SER:HG	1.67	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
1:A:334:ASP:HA	1:A:337:PHE:CD2	2.56	0.41
1:A:164:ARG:HH11	1:A:164:ARG:HG2	1.86	0.41
2:F:1351:PRO:HA	2:F:1354:ARG:HH11	1.86	0.41
2:B:1416:LYS:O	2:B:1420:GLN:HB2	2.21	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:D:1416:LYS:O	2:D:1420:GLN:HB2	2.21	0.40
2:B:1273:TYR:HB3	2:B:1394:PHE:CD1	2.56	0.40
1:G:344:VAL:HG11	1:G:539:ILE:HG21	2.03	0.40
1:G:192:SER:C	1:G:193:LEU:HD23	2.42	0.40
2:D:1340:LYS:HD3	2:D:1383:TYR:CG	2.57	0.40
1:A:536:ASP:OD1	1:A:586:ARG:NH2	2.54	0.40
1:E:207:LYS:HG2	1:E:208:SER:N	2.36	0.40

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:387:GLU:O	1:A:391:ASN:ND2	2.54	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
1:G:199:PRO:CG	1:G:200:GLU:N	2.85	0.40
2:D:1414:LYS:HZ3	2:D:1418:LYS:HD3	1.81	0.40
1:G:308:ASN:OD1	1:G:313:LYS:O	2.40	0.40
2:D:1405:LEU:HA	2:D:1408:LEU:HD23	2.03	0.40
1:E:362:ASP:O	1:E:366:VAL:HG23	2.21	0.40
1:A:506:ARG:N	1:A:506:ARG:HD2	2.37	0.40
1:G:185:ARG:CG	1:G:185:ARG:NH1	2.81	0.40
2:B:1354:ARG:HA	2:B:1354:ARG:HD3	1.91	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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%)	14	24
1	C	435/598 (73%)	409 (94%)	18 (4%)	8 (2%)	11	18
1	E	435/598 (73%)	414 (95%)	16 (4%)	5 (1%)	17	31
1	G	430/598 (72%)	400 (93%)	19 (4%)	11 (3%)	7	10
2	B	171/180 (95%)	163 (95%)	7 (4%)	1 (1%)	30	50
2	D	176/180 (98%)	166 (94%)	8 (4%)	2 (1%)	17	31
2	F	174/180 (97%)	164 (94%)	7 (4%)	3 (2%)	11	19
2	H	177/180 (98%)	168 (95%)	8 (4%)	1 (1%)	30	50
All	All	2438/3112 (78%)	2296 (94%)	105 (4%)	37 (2%)	13	22

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 ⓘ

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%)	18	33
1	C	389/527 (74%)	356 (92%)	33 (8%)	13	25
1	E	387/527 (73%)	350 (90%)	37 (10%)	10	19
1	G	385/527 (73%)	347 (90%)	38 (10%)	10	18
2	B	162/168 (96%)	147 (91%)	15 (9%)	11	21
2	D	167/168 (99%)	152 (91%)	15 (9%)	12	22
2	F	165/168 (98%)	149 (90%)	16 (10%)	10	19
2	H	168/168 (100%)	154 (92%)	14 (8%)	14	26
All	All	2212/2780 (80%)	2016 (91%)	196 (9%)	12	23

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

*Continued on next page...*



*Continued from previous page...*

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

*Continued on next page...*

*Continued from previous page...*

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

*Continued on next page...*

*Continued from previous page...*

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

*Continued on next page...*

*Continued from previous page...*

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

*Continued on next page...*

*Continued from previous page...*

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

Some 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

*Continued on next page...*

*Continued from previous page...*

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 ⓘ

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

### 5.6 Ligand geometry ⓘ

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 ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	442/598 (73%)	-0.01	13 (2%) 55 60	18, 42, 87, 110	0
1	C	441/598 (73%)	-0.07	16 (3%) 46 51	16, 35, 86, 106	0
1	E	439/598 (73%)	-0.08	8 (1%) 71 75	20, 38, 86, 105	0
1	G	436/598 (72%)	0.08	10 (2%) 64 67	31, 53, 91, 115	0
2	B	173/180 (96%)	0.51	19 (10%) 7 7	15, 55, 104, 116	0
2	D	178/180 (98%)	0.28	15 (8%) 14 14	17, 50, 96, 110	0
2	F	176/180 (97%)	0.09	8 (4%) 37 42	26, 48, 89, 104	0
2	H	179/180 (99%)	0.98	39 (21%) 1 1	39, 71, 105, 118	0
All	All	2464/3112 (79%)	0.12	128 (5%) 31 35	15, 46, 94, 118	0

All (128) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	1300	GLY	8.6
1	C	152	SER	8.5
1	G	580	ALA	7.7
2	D	1300	GLY	6.6
2	H	1412	HIS	6.1
2	B	1299	SER	5.6
2	B	1410	THR	5.4
1	G	582	ASP	5.3
2	D	1408	LEU	5.2
2	F	1267	LEU	5.2
2	F	1266	GLN	5.1
2	H	1300	GLY	5.0
2	B	1409	THR	4.8
2	H	1301	THR	4.7
2	H	1407	LYS	4.7
2	H	1405	LEU	4.6

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	C	153	PRO	4.5
2	H	1410	THR	4.5
2	D	1417	LEU	4.4
1	A	491	THR	4.4
2	D	1409	THR	4.3
2	H	1266	GLN	4.3
1	E	335	ALA	4.2
1	G	202	LEU	4.1
2	H	1413	GLU	4.1
2	F	1313	ILE	4.1
2	D	1299	SER	4.1
2	H	1411	ASP	4.0
2	H	1409	THR	3.9
1	A	332	GLU	3.9
1	E	332	GLU	3.8
2	B	1417	LEU	3.8
1	C	311	GLY	3.7
1	A	585	GLU	3.7
2	H	1287	GLY	3.6
2	F	1412	HIS	3.5
2	H	1421	PHE	3.5
2	B	1440	PHE	3.4
1	C	198	CYS	3.4
1	C	584	ALA	3.4
1	C	312	ARG	3.3
1	G	585	GLU	3.3
2	B	1414	LYS	3.3
2	H	1440	PHE	3.3
1	E	585	GLU	3.3
2	D	1413	GLU	3.3
1	A	582	ASP	3.3
2	F	1440	PHE	3.3
1	E	206	TYR	3.2
2	B	1411	ASP	3.2
2	D	1405	LEU	3.2
2	H	1316	LYS	3.2
2	D	1421	PHE	3.2
1	C	585	GLU	3.2
2	H	1267	LEU	3.1
2	H	1415	ASP	3.1
2	B	1412	HIS	3.1
2	D	1412	HIS	3.1

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
2	B	1298	GLY	3.1
2	D	1301	THR	3.1
2	B	1422	PHE	3.1
2	D	1410	THR	3.0
2	F	1410	THR	2.9
2	H	1441	LEU	2.9
1	A	187	GLY	2.9
2	D	1308	TYR	2.9
2	H	1308	TYR	2.8
1	A	489	SER	2.8
2	B	1419	LYS	2.8
1	C	151	PHE	2.8
2	B	1415	ASP	2.8
1	A	581	ALA	2.8
1	C	202	LEU	2.7
2	H	1268	THR	2.7
2	H	1313	ILE	2.7
2	H	1292	TYR	2.7
1	G	581	ALA	2.7
1	A	336	ASP	2.7
2	B	1301	THR	2.7
1	A	335	ALA	2.7
1	G	187	GLY	2.7
1	E	336	ASP	2.6
1	C	583	GLY	2.6
1	G	584	ALA	2.6
2	B	1303	MET	2.6
2	B	1311	SER	2.5
2	H	1408	LEU	2.5
1	E	581	ALA	2.5
2	F	1439	GLN	2.5
2	H	1422	PHE	2.5
2	H	1291	ILE	2.5
2	H	1314	ASP	2.4
2	H	1416	LYS	2.4
2	H	1299	SER	2.4
1	C	201	ALA	2.4
2	H	1443	ARG	2.4
2	H	1269	ASP	2.4
1	A	393	LEU	2.4
1	A	189	GLY	2.3
1	G	336	ASP	2.3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
2	H	1444	SER	2.3
1	C	447	ARG	2.3
1	C	188	ALA	2.3
2	B	1421	PHE	2.3
2	D	1407	LYS	2.3
2	H	1280	LYS	2.3
1	G	200	GLU	2.2
2	H	1303	MET	2.2
2	H	1304	GLU	2.2
2	H	1419	LYS	2.2
1	C	181	SER	2.2
1	A	448	GLU	2.2
2	H	1373	ALA	2.2
1	E	331	THR	2.2
2	F	1314	ASP	2.2
2	B	1305	PRO	2.1
1	C	154	SER	2.1
1	G	201	ALA	2.1
1	E	330	PRO	2.1
2	H	1284	PRO	2.1
2	H	1414	LYS	2.1
2	H	1417	LEU	2.1
2	B	1402	GLU	2.1
1	A	333	GLU	2.1
2	D	1298	GLY	2.1
2	D	1314	ASP	2.1
1	C	580	ALA	2.0
2	H	1296	PHE	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 carbohydrates 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. LLDF column lists the quality of electron

density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	ZN	B	1502	1/1	1.00	0.14	0.99	37,37,37,37	0
3	ZN	D	1502	1/1	1.00	0.10	-0.85	43,43,43,43	0
3	ZN	F	1502	1/1	0.96	0.10	-0.99	62,62,62,62	0
3	ZN	F	1501	1/1	0.99	0.07	-1.68	53,53,53,53	0
3	ZN	H	1502	1/1	0.98	0.09	-1.71	64,64,64,64	0
3	ZN	D	1501	1/1	0.99	0.06	-1.93	66,66,66,66	0
3	ZN	H	1501	1/1	0.93	0.05	-2.18	88,88,88,88	0
3	ZN	B	1501	1/1	0.96	0.04	-2.97	82,82,82,82	0

## 6.5 Other polymers

There are no such residues in this entry.