



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 01:30 am GMT

PDB ID : 3SCI
Title : Crystal structure of spike protein receptor-binding domain from a predicted SARS coronavirus human strain complexed with human receptor ACE2
Authors : Wu, K.; Peng, G.; Wilken, M.; Geraghty, R.; Li, F.
Deposited on : 2011-06-07
Resolution : 2.90 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

<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
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : recalc28949

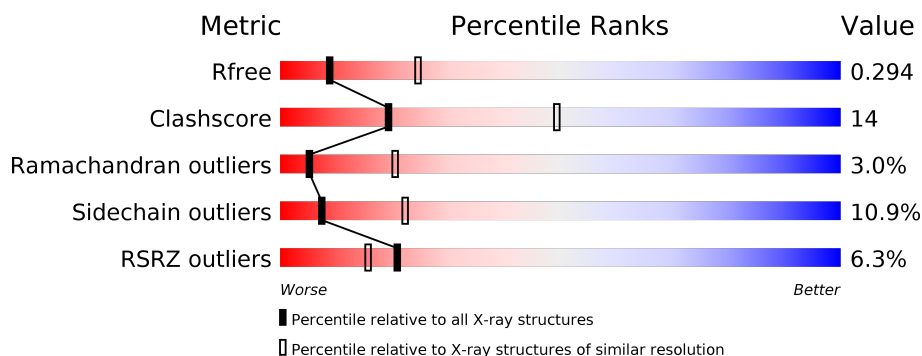
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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}	100719	1586 (2.90-2.90)
Clashscore	112137	1807 (2.90-2.90)
Ramachandran outliers	110173	1768 (2.90-2.90)
Sidechain outliers	110143	1770 (2.90-2.90)
RSRZ outliers	101464	1596 (2.90-2.90)

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 ≥ 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	603	<div> <div>2%</div> <div> <div></div> <div>62%</div> <div>32%</div> <div>5%</div> </div> </div>
1	B	603	<div> <div>6%</div> <div> <div></div> <div>63%</div> <div>32%</div> <div>5%</div> </div> </div>
2	E	228	<div> <div>10%</div> <div> <div></div> <div>51%</div> <div>18%</div> <div>8%</div> <div>24%</div> </div> </div>
2	F	228	<div> <div>11%</div> <div> <div></div> <div>44%</div> <div>29%</div> <div>•</div> <div>24%</div> </div> </div>

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

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	CL	A	902	-	-	-	X
4	CL	B	902	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 12552 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 Angiotensin-converting enzyme 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	597	Total	C	N	O	S	0	0	0
			4870	3115	806	920	29			
1	B	597	Total	C	N	O	S	0	0	0
			4870	3115	806	920	29			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	616	HIS	-	EXPRESSION TAG	UNP Q9BYF1
A	617	HIS	-	EXPRESSION TAG	UNP Q9BYF1
A	618	HIS	-	EXPRESSION TAG	UNP Q9BYF1
A	619	HIS	-	EXPRESSION TAG	UNP Q9BYF1
A	620	HIS	-	EXPRESSION TAG	UNP Q9BYF1
A	621	HIS	-	EXPRESSION TAG	UNP Q9BYF1
B	616	HIS	-	EXPRESSION TAG	UNP Q9BYF1
B	617	HIS	-	EXPRESSION TAG	UNP Q9BYF1
B	618	HIS	-	EXPRESSION TAG	UNP Q9BYF1
B	619	HIS	-	EXPRESSION TAG	UNP Q9BYF1
B	620	HIS	-	EXPRESSION TAG	UNP Q9BYF1
B	621	HIS	-	EXPRESSION TAG	UNP Q9BYF1

- Molecule 2 is a protein called Spike glycoprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	174	Total	C	N	O	S	0	0	0
			1404	912	228	257	7			
2	F	174	Total	C	N	O	S	0	0	0
			1404	912	228	257	7			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	442	PHE	TYR	CONFLICT	UNP P59594
E	472	PHE	LEU	CONFLICT	UNP P59594
E	528	HIS	-	EXPRESSION TAG	UNP P59594
E	529	HIS	-	EXPRESSION TAG	UNP P59594
E	530	HIS	-	EXPRESSION TAG	UNP P59594
E	531	HIS	-	EXPRESSION TAG	UNP P59594
E	532	HIS	-	EXPRESSION TAG	UNP P59594
E	533	HIS	-	EXPRESSION TAG	UNP P59594
F	442	PHE	TYR	CONFLICT	UNP P59594
F	472	PHE	LEU	CONFLICT	UNP P59594
F	528	HIS	-	EXPRESSION TAG	UNP P59594
F	529	HIS	-	EXPRESSION TAG	UNP P59594
F	530	HIS	-	EXPRESSION TAG	UNP P59594
F	531	HIS	-	EXPRESSION TAG	UNP P59594
F	532	HIS	-	EXPRESSION TAG	UNP P59594
F	533	HIS	-	EXPRESSION TAG	UNP P59594

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

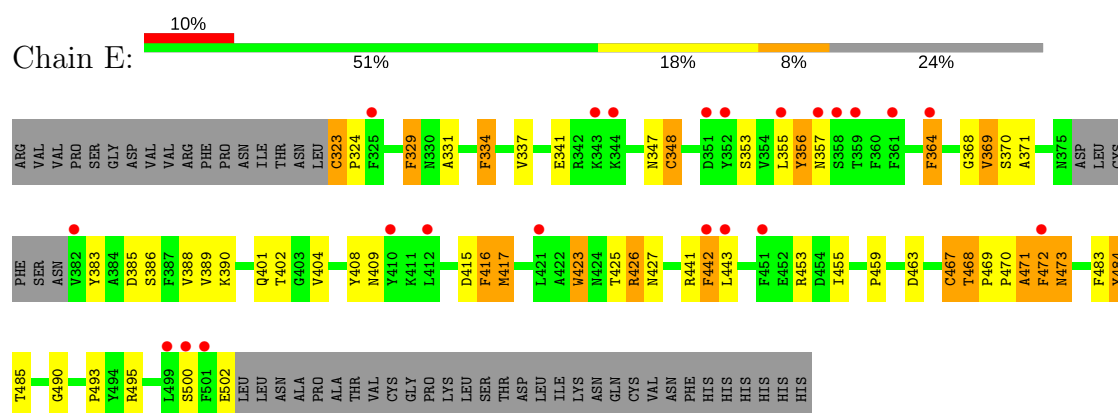
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total Zn 1 1	0	0
3	A	1	Total Zn 1 1	0	0

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

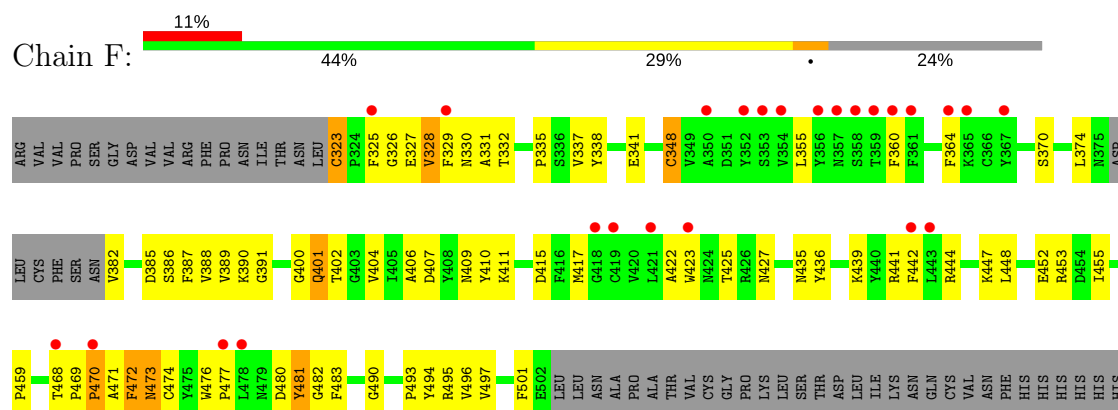
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total Cl 1 1	0	0
4	A	1	Total Cl 1 1	0	0



• Molecule 2: Spike glycoprotein



• Molecule 2: Spike glycoprotein



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	81.36Å 118.33Å 111.94Å 90.00° 93.06° 90.00°	Depositor
Resolution (Å)	47.24 – 2.90 47.24 – 2.90	Depositor EDS
% Data completeness (in resolution range)	85.5 (47.24-2.90) 84.9 (47.24-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.54 (at 2.91Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.226 , 0.283 0.241 , 0.294	Depositor DCC
R_{free} test set	2003 reflections (5.28%)	DCC
Wilson B-factor (Å ²)	77.7	Xtriage
Anisotropy	0.124	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 32.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	12552	wwPDB-VP
Average B, all atoms (Å ²)	79.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.62% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 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, CL

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	0.50	0/5007	0.62	0/6803
1	B	0.52	1/5007 (0.0%)	0.62	0/6803
2	E	0.52	0/1450	0.66	0/1975
2	F	0.49	0/1450	0.61	0/1975
All	All	0.51	1/12914 (0.0%)	0.62	0/17556

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	105	SER	CB-OG	7.02	1.51	1.42

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	290	ASN	Peptide

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	4870	0	4643	133	0
1	B	4870	0	4643	142	0
2	E	1404	0	1325	37	0
2	F	1404	0	1325	42	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
All	All	12552	0	11936	354	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 14.

All (354) 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:B:366:MET:HE1	1:B:441:LYS:HE3	1.43	0.98
1:B:24:GLN:HG3	1:B:83:TYR:HE2	1.29	0.95
1:B:323:MET:HA	1:B:323:MET:HE3	1.48	0.95
2:E:409:ASN:HD21	2:E:441:ARG:H	1.15	0.95
2:F:335:PRO:HG3	2:F:341:GLU:HG2	1.47	0.94
1:B:245:ARG:HH21	1:B:245:ARG:HG2	1.34	0.91
1:B:393:ARG:O	1:B:394:ASN:HB2	1.73	0.89
1:A:122:THR:O	1:A:126:ILE:HG22	1.80	0.82
1:A:245:ARG:HG2	1:A:245:ARG:HH21	1.45	0.81
1:A:132:VAL:HG12	1:A:171:GLU:HG3	1.66	0.76
1:A:309:LYS:HD2	1:A:328:TRP:CH2	2.23	0.74
2:E:472:PHE:O	2:E:473:ASN:HB2	1.88	0.74
2:E:453:ARG:NH1	2:E:455:ILE:HD11	2.04	0.72
1:A:229:THR:HG23	1:A:516:TYR:OH	1.90	0.71
2:F:425:THR:HG21	2:F:495:ARG:HG3	1.73	0.71
1:B:262:LEU:O	1:B:487:VAL:HG13	1.91	0.71
1:A:320:LEU:HD13	1:A:380:GLN:HG2	1.72	0.69
1:A:285:PHE:HE1	1:A:436:ILE:HG21	1.56	0.69
2:F:439:LYS:HE2	2:F:480:ASP:OD2	1.92	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:457:GLU:OE2	1:A:512:PHE:N	2.26	0.69
1:B:323:MET:HA	1:B:323:MET:CE	2.23	0.69
1:B:20:THR:HG23	1:B:23:GLU:HB2	1.75	0.69
1:B:366:MET:CE	1:B:441:LYS:HE3	2.19	0.69
1:B:245:ARG:NH1	1:B:605:GLY:O	2.27	0.68
1:A:560:LEU:O	1:A:563:SER:HB3	1.93	0.68
1:B:478:TRP:O	1:B:482:ARG:HB2	1.93	0.68
1:B:122:THR:O	1:B:126:ILE:HG22	1.94	0.67
1:B:320:LEU:HD13	1:B:380:GLN:HG2	1.76	0.67
1:B:407:ILE:HD11	1:B:522:GLN:HA	1.76	0.67
1:B:580:ASN:HD21	1:B:582:ARG:CZ	2.08	0.67
1:B:252:TYR:CE2	1:B:266:LEU:HD22	2.30	0.67
2:E:409:ASN:ND2	2:E:441:ARG:H	1.91	0.67
1:A:450:LEU:HD21	1:A:519:THR:HG21	1.76	0.66
1:B:139:GLN:HG3	1:B:140:GLU:H	1.60	0.66
2:E:353:SER:HA	2:E:356:TYR:HB2	1.76	0.66
1:A:142:LEU:HD23	1:A:143:LEU:HD12	1.78	0.66
1:A:21:ILE:HD13	1:A:21:ILE:H	1.61	0.65
1:B:549:GLU:H	1:B:549:GLU:CD	1.97	0.65
1:A:47:SER:HA	1:A:62:MET:HG3	1.77	0.65
1:A:201:ASP:O	1:A:219:ARG:HD2	1.96	0.64
1:A:271:TRP:CE2	1:A:503:LEU:HD23	2.32	0.64
1:A:511:SER:O	1:A:514:ARG:HD2	1.98	0.64
1:A:21:ILE:HA	1:A:24:GLN:HG2	1.80	0.63
1:A:494:ASP:OD2	1:A:496:THR:HG22	1.98	0.63
1:B:459:TRP:O	1:B:463:VAL:HG23	1.97	0.63
1:A:142:LEU:HD23	1:A:143:LEU:H	1.63	0.63
1:B:21:ILE:HA	1:B:24:GLN:HG2	1.81	0.63
1:B:418:LEU:O	1:B:421:ILE:HG22	1.99	0.63
1:B:24:GLN:HG3	1:B:83:TYR:CE2	2.22	0.62
2:E:337:VAL:HG22	2:E:388:VAL:O	1.99	0.62
1:A:485:VAL:HG12	1:A:487:VAL:HG13	1.82	0.62
2:E:459:PRO:HB2	2:E:467:CYS:CB	2.30	0.61
1:B:245:ARG:NH2	1:B:245:ARG:HG2	2.10	0.61
1:B:351:LEU:HB2	1:B:355:ASP:HB3	1.81	0.61
1:A:271:TRP:CD2	1:A:503:LEU:HD23	2.35	0.61
1:A:126:ILE:HA	1:A:129:THR:HG22	1.84	0.60
1:A:514:ARG:HG2	1:A:515:TYR:N	2.16	0.60
1:A:438:PHE:O	1:A:441:LYS:HB3	2.01	0.60
1:B:249:MET:HG2	1:B:256:ILE:HB	1.83	0.60
1:A:378:HIS:CE1	1:A:402:GLU:OE1	2.55	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:472:PHE:O	2:F:473:ASN:HB2	2.01	0.60
1:B:90:ASN:O	1:B:92:THR:N	2.35	0.59
1:A:269:ASP:OD2	1:A:272:GLY:N	2.31	0.59
2:E:341:GLU:O	2:E:385:ASP:HA	2.02	0.59
1:B:440:LEU:HD13	1:B:440:LEU:C	2.23	0.59
2:E:364:PHE:O	2:E:364:PHE:HD2	1.86	0.59
1:A:499:ASP:O	1:A:502:SER:HB3	2.03	0.59
1:A:457:GLU:HG2	1:A:460:ARG:HH11	1.68	0.58
1:B:520:LEU:HD22	1:B:579:MET:CE	2.33	0.58
1:A:234:LYS:HB2	1:A:235:PRO:HD3	1.85	0.58
1:B:180:TYR:HA	1:B:183:TYR:HB3	1.85	0.58
1:A:460:ARG:NE	1:A:506:VAL:HG22	2.18	0.58
1:A:514:ARG:HG2	1:A:515:TYR:H	1.68	0.58
1:B:275:TRP:HB3	1:B:278:LEU:HD22	1.84	0.58
2:E:426:ARG:HD3	2:E:485:THR:O	2.04	0.58
2:F:444:ARG:HH12	2:F:447:LYS:C	2.07	0.58
2:F:469:PRO:HG3	2:F:476:TRP:CZ2	2.40	0.57
2:F:390:LYS:HG2	2:F:490:GLY:O	2.05	0.57
1:A:501:ALA:O	1:A:507:SER:HB3	2.04	0.57
1:A:460:ARG:NH2	1:A:510:TYR:O	2.37	0.57
1:B:305:GLN:O	1:B:309:LYS:HB2	2.05	0.57
1:B:407:ILE:CD1	1:B:522:GLN:HA	2.34	0.56
1:A:394:ASN:HB3	1:A:562:LYS:HG3	1.88	0.56
2:F:435:ASN:O	2:F:482:GLY:HA2	2.05	0.56
1:A:225:ASP:O	1:A:229:THR:HG22	2.05	0.56
1:B:226:VAL:O	1:B:229:THR:HG22	2.04	0.56
1:A:591:LEU:HG	1:A:595:LEU:CD2	2.34	0.56
1:B:155:SER:O	1:B:161:ARG:HD2	2.05	0.56
1:A:199:TYR:O	1:A:202:TYR:HB3	2.05	0.56
1:A:489:GLU:HG2	1:A:613:TYR:HE2	1.69	0.56
2:F:406:ALA:HA	2:F:410:TYR:O	2.05	0.56
1:B:407:ILE:HB	1:B:408:MET:CE	2.36	0.56
1:B:47:SER:HA	1:B:62:MET:HG3	1.87	0.56
1:A:402:GLU:HB3	1:A:518:ARG:HD2	1.86	0.56
1:A:456:LEU:CD2	1:A:477:TRP:HH2	2.19	0.55
1:B:457:GLU:HG2	1:B:512:PHE:HB3	1.88	0.55
2:E:472:PHE:O	2:E:473:ASN:CB	2.54	0.55
2:F:471:ALA:O	2:F:473:ASN:N	2.39	0.55
2:E:409:ASN:HD21	2:E:441:ARG:N	1.95	0.55
1:B:483:GLU:HA	1:B:606:TRP:HE1	1.71	0.55
1:B:275:TRP:O	1:B:278:LEU:HB2	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:385:TYR:O	1:B:393:ARG:HG2	2.07	0.55
1:A:446:ILE:HD13	1:A:523:PHE:HZ	1.72	0.55
1:B:574:VAL:HG23	1:B:575:GLY:N	2.22	0.55
2:E:390:LYS:HG2	2:E:490:GLY:O	2.07	0.54
1:B:132:VAL:O	1:B:141:CYS:HB3	2.07	0.54
1:A:456:LEU:HD22	1:A:477:TRP:HH2	1.71	0.54
2:E:484:TYR:CD1	2:E:484:TYR:N	2.75	0.54
1:A:555:PHE:HA	1:A:558:LEU:HB2	1.88	0.54
1:B:126:ILE:HD11	1:B:175:GLN:HB2	1.90	0.54
1:B:41:TYR:CE2	1:B:45:LEU:HD11	2.42	0.54
1:B:526:GLN:HE21	1:B:526:GLN:HA	1.72	0.54
1:B:323:MET:HE1	1:B:379:ILE:HG21	1.89	0.54
1:B:489:GLU:N	1:B:489:GLU:OE1	2.34	0.54
1:B:574:VAL:HG23	1:B:576:ALA:H	1.73	0.54
1:A:457:GLU:HG2	1:A:460:ARG:NH1	2.22	0.54
1:B:520:LEU:HD22	1:B:579:MET:HE1	1.89	0.53
2:E:442:PHE:CE2	2:E:443:LEU:HG	2.43	0.53
1:A:166:GLU:OE1	1:A:493:HIS:HE1	1.91	0.53
1:B:446:ILE:HD12	1:B:522:GLN:HE22	1.73	0.53
1:B:574:VAL:HG23	1:B:575:GLY:H	1.73	0.53
2:F:409:ASN:HD21	2:F:441:ARG:H	1.55	0.53
1:B:225:ASP:O	1:B:229:THR:HB	2.08	0.53
1:B:381:TYR:CD2	1:B:558:LEU:HG	2.43	0.53
1:A:181:GLU:O	1:A:184:VAL:HG22	2.08	0.53
1:B:294:THR:HG23	1:B:365:THR:HA	1.91	0.53
1:A:346:PRO:HB3	1:A:360:MET:HG3	1.91	0.53
1:A:393:ARG:O	1:A:394:ASN:HB2	2.09	0.53
1:B:270:MET:HB3	1:B:271:TRP:CE3	2.44	0.53
1:A:285:PHE:CE1	1:A:436:ILE:HG21	2.41	0.53
1:A:457:GLU:HG3	1:A:512:PHE:HB3	1.90	0.53
1:A:555:PHE:O	1:A:559:ARG:HG2	2.08	0.53
1:B:366:MET:O	1:B:369:PHE:HB3	2.09	0.53
1:A:233:ILE:HD11	1:A:581:VAL:HG21	1.91	0.52
1:B:126:ILE:HA	1:B:129:THR:HG22	1.91	0.52
1:A:169:ARG:O	1:A:173:GLY:HA3	2.09	0.52
1:A:323:MET:CE	1:A:323:MET:HA	2.39	0.52
2:F:400:GLY:O	2:F:401:GLN:HB2	2.09	0.52
2:F:422:ALA:HA	2:F:495:ARG:O	2.10	0.52
1:B:480:MET:HA	1:B:483:GLU:OE2	2.09	0.52
1:A:24:GLN:HG3	1:A:83:TYR:HE2	1.73	0.52
1:B:152:MET:HG3	1:B:270:MET:HA	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:325:PHE:C	2:F:327:GLU:H	2.12	0.52
1:A:96:GLN:HE21	1:A:391:LEU:HB2	1.75	0.52
1:B:239:HIS:CE1	1:B:596:LYS:HA	2.45	0.51
1:A:330:ASN:HB3	1:A:357:ARG:NE	2.25	0.51
1:A:90:ASN:O	1:A:92:THR:N	2.43	0.51
1:A:166:GLU:OE1	1:A:493:HIS:CE1	2.63	0.51
1:B:509:ASP:C	1:B:509:ASP:OD1	2.49	0.51
2:F:388:VAL:CG2	2:F:495:ARG:HG2	2.41	0.51
1:A:454:TYR:OH	1:A:458:LYS:NZ	2.44	0.51
1:A:524:GLN:NE2	1:A:580:ASN:H	2.09	0.51
1:B:271:TRP:NE1	1:B:502:SER:O	2.32	0.51
1:A:418:LEU:HB3	1:A:424:LEU:HB2	1.93	0.51
1:A:316:VAL:HA	1:A:320:LEU:O	2.09	0.51
1:B:94:LYS:O	1:B:98:GLN:HB2	2.10	0.51
2:F:337:VAL:HG13	2:F:387:PHE:CD1	2.46	0.51
2:F:435:ASN:OD1	2:F:436:TYR:N	2.44	0.51
2:F:483:PHE:CD2	2:F:493:PRO:HD3	2.45	0.51
1:A:524:GLN:CD	1:A:580:ASN:H	2.14	0.50
2:E:388:VAL:CG2	2:E:495:ARG:HG2	2.41	0.50
1:B:294:THR:O	1:B:298:VAL:HG23	2.12	0.50
1:B:446:ILE:CD1	1:B:522:GLN:HE22	2.24	0.50
2:F:323:CYS:N	2:F:348:CYS:SG	2.84	0.50
1:A:142:LEU:HD22	1:A:146:PRO:O	2.12	0.50
1:A:450:LEU:HD21	1:A:519:THR:CG2	2.41	0.50
1:A:411:SER:OG	1:A:544:ILE:HG12	2.12	0.49
1:B:323:MET:HE1	1:B:379:ILE:CG2	2.42	0.49
1:B:318:VAL:O	1:B:548:THR:HA	2.13	0.49
1:A:468:ILE:HD12	1:A:476:LYS:HG3	1.94	0.49
1:A:97:LEU:O	1:A:101:GLN:HG2	2.13	0.49
1:A:153:ALA:HA	1:A:268:GLY:O	2.14	0.48
1:A:526:GLN:O	1:A:530:CYS:SG	2.71	0.48
1:B:288:LYS:HB3	1:B:289:PRO:CD	2.43	0.48
2:E:337:VAL:HG21	2:E:389:VAL:HG12	1.94	0.48
2:F:327:GLU:O	2:F:331:ALA:HB2	2.12	0.48
2:F:391:GLY:HA2	2:F:494:TYR:CD1	2.48	0.48
1:A:204:ARG:HD2	1:A:219:ARG:O	2.13	0.48
1:A:432:ASN:HD22	1:A:433:GLU:N	2.12	0.48
1:A:175:GLN:O	1:A:178:PRO:HD2	2.13	0.48
1:B:275:TRP:HB3	1:B:278:LEU:CD2	2.43	0.48
2:E:459:PRO:HB2	2:E:467:CYS:HB3	1.95	0.48
2:F:453:ARG:CZ	2:F:455:ILE:HD11	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:265:HIS:ND1	1:A:490:PRO:HG3	2.28	0.48
2:F:472:PHE:O	2:F:473:ASN:CB	2.62	0.48
1:A:335:ASP:HB2	1:A:361:CYS:HB3	1.96	0.48
1:B:450:LEU:HA	1:B:450:LEU:HD12	1.61	0.48
2:E:368:GLY:O	2:E:369:VAL:HG13	2.14	0.47
2:E:388:VAL:HG22	2:E:495:ARG:HG2	1.96	0.47
1:A:433:GLU:O	1:A:436:ILE:HG22	2.15	0.47
1:B:291:ILE:HG22	1:B:291:ILE:O	2.13	0.47
2:E:364:PHE:CD2	2:E:364:PHE:O	2.66	0.47
1:B:238:GLU:O	1:B:241:HIS:HB3	2.14	0.47
1:B:524:GLN:NE2	1:B:580:ASN:H	2.12	0.47
2:F:406:ALA:O	2:F:411:LYS:HD2	2.14	0.47
1:A:338:ASN:HA	1:A:341:LYS:HE3	1.97	0.47
1:B:143:LEU:O	1:B:148:LEU:HB2	2.15	0.47
1:B:312:GLU:HG3	1:B:323:MET:HG2	1.96	0.47
2:E:467:CYS:O	2:E:468:THR:HG23	2.14	0.47
2:F:341:GLU:O	2:F:385:ASP:HA	2.14	0.47
1:A:245:ARG:HG2	1:A:245:ARG:NH2	2.22	0.47
1:A:245:ARG:NH1	1:A:605:GLY:O	2.48	0.47
1:A:204:ARG:HG2	1:A:222:LEU:HD23	1.95	0.47
1:A:338:ASN:O	1:A:339:VAL:HB	2.15	0.47
1:B:208:GLU:HG2	1:B:209:VAL:N	2.30	0.47
1:B:220:GLY:HA2	1:B:223:ILE:HD12	1.96	0.47
1:B:378:HIS:CE1	1:B:402:GLU:OE1	2.68	0.47
1:A:167:SER:O	1:A:171:GLU:HG2	2.15	0.47
1:A:233:ILE:HD11	1:A:581:VAL:CG2	2.44	0.47
1:B:499:ASP:N	1:B:500:PRO:HD2	2.30	0.47
1:B:589:GLU:HA	1:B:589:GLU:OE1	2.15	0.47
1:A:323:MET:HE1	1:A:379:ILE:HG21	1.97	0.47
1:B:407:ILE:HB	1:B:408:MET:HE1	1.97	0.47
1:A:578:ASN:ND2	1:A:579:MET:H	2.13	0.47
1:A:88:ILE:HB	1:A:94:LYS:HE3	1.96	0.47
1:B:115:ARG:O	1:B:119:ILE:HG12	2.14	0.47
1:A:414:THR:OG1	1:A:543:ASP:HB2	2.15	0.47
1:B:369:PHE:O	1:B:373:HIS:HD2	1.98	0.47
1:B:389:PRO:O	1:B:390:PHE:C	2.54	0.47
1:B:414:THR:O	1:B:418:LEU:HD22	2.14	0.47
1:A:47:SER:HA	1:A:62:MET:CG	2.44	0.46
1:A:554:LEU:HG	1:A:558:LEU:HD22	1.97	0.46
1:B:311:ALA:O	1:B:314:PHE:HB3	2.16	0.46
1:B:407:ILE:HB	1:B:408:MET:HE2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:493:HIS:HD2	1:B:499:ASP:OD1	1.97	0.46
2:F:329:PHE:C	2:F:331:ALA:H	2.17	0.46
1:A:90:ASN:HD22	1:A:93:VAL:HG13	1.80	0.46
1:B:389:PRO:HG2	1:B:392:LEU:HD22	1.96	0.46
2:E:423:TRP:CD1	2:E:423:TRP:N	2.84	0.46
2:F:469:PRO:HA	2:F:470:PRO:HA	1.74	0.46
1:A:249:MET:HE1	1:A:258:PRO:HG3	1.98	0.46
1:A:125:THR:O	1:A:129:THR:N	2.43	0.46
1:A:305:GLN:O	1:A:309:LYS:HB2	2.15	0.46
1:B:306:ARG:O	1:B:310:GLU:HB2	2.15	0.46
1:A:326:GLY:O	1:A:330:ASN:HB2	2.16	0.46
1:B:269:ASP:OD2	1:B:272:GLY:N	2.49	0.46
2:E:383:TYR:HE1	2:E:502:GLU:HB3	1.81	0.46
1:A:257:SER:HB2	1:A:610:TRP:CE2	2.50	0.46
1:A:503:LEU:O	1:A:504:PHE:C	2.54	0.46
1:A:456:LEU:HD22	1:A:477:TRP:CH2	2.49	0.46
1:B:184:VAL:O	1:B:188:ASN:HB2	2.16	0.45
1:B:97:LEU:O	1:B:101:GLN:HG2	2.16	0.45
1:A:245:ARG:HB2	1:A:262:LEU:HD21	1.97	0.45
1:A:50:TYR:C	1:A:52:THR:H	2.20	0.45
1:B:249:MET:CG	1:B:256:ILE:HB	2.46	0.45
1:B:482:ARG:O	1:B:486:GLY:HA2	2.17	0.45
2:E:334:PHE:CE2	2:E:386:SER:HB2	2.51	0.45
1:A:516:TYR:O	1:A:519:THR:HG22	2.17	0.45
1:B:188:ASN:HD21	1:B:464:PHE:HA	1.82	0.45
2:E:329:PHE:C	2:E:331:ALA:H	2.21	0.45
1:A:187:LYS:HG2	1:A:199:TYR:CE2	2.52	0.44
1:A:545:SER:O	1:A:547:SER:N	2.50	0.44
1:B:468:ILE:HG22	1:B:473:TRP:HD1	1.81	0.44
2:F:404:VAL:H	2:F:407:ASP:HB2	1.83	0.44
2:F:388:VAL:HG22	2:F:495:ARG:HA	2.00	0.44
2:F:385:ASP:O	2:F:497:VAL:HA	2.17	0.44
1:B:261:CYS:HB2	1:B:488:VAL:HG13	1.99	0.44
1:B:309:LYS:HD2	1:B:328:TRP:CH2	2.53	0.44
1:A:517:THR:O	1:A:518:ARG:C	2.56	0.44
1:B:240:LEU:O	1:B:244:VAL:HG13	2.18	0.44
1:B:526:GLN:NE2	1:B:526:GLN:HA	2.33	0.44
2:E:324:PRO:HD3	2:E:348:CYS:SG	2.58	0.44
1:A:180:TYR:O	1:A:184:VAL:HG13	2.17	0.44
1:B:139:GLN:HG3	1:B:140:GLU:N	2.30	0.44
1:B:251:ALA:O	1:B:253:PRO:HD3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:469:PRO:HA	2:E:470:PRO:HA	1.74	0.44
2:F:471:ALA:O	2:F:474:CYS:N	2.42	0.44
1:B:440:LEU:CD1	1:B:444:LEU:HD22	2.47	0.43
1:B:526:GLN:O	1:B:527:GLU:C	2.55	0.43
1:B:503:LEU:HD23	1:B:504:PHE:N	2.32	0.43
1:B:553:LYS:HE3	1:B:573:VAL:HA	2.00	0.43
1:B:557:MET:HA	1:B:560:LEU:HD22	2.00	0.43
2:E:404:VAL:O	2:E:408:TYR:HB2	2.18	0.43
2:E:416:PHE:O	2:E:417:MET:CB	2.66	0.43
1:A:126:ILE:HG23	1:A:176:LEU:HD21	2.00	0.43
1:A:320:LEU:HB3	1:A:321:PRO:HD2	1.99	0.43
1:B:589:GLU:HB2	1:B:590:PRO:HD3	1.99	0.43
2:F:448:LEU:HD22	2:F:452:GLU:HG2	2.01	0.43
1:B:183:TYR:O	1:B:187:LYS:HB2	2.19	0.43
1:B:494:ASP:OD2	1:B:494:ASP:N	2.47	0.43
1:B:147:GLY:O	1:B:151:ILE:HG12	2.19	0.43
1:B:275:TRP:CD1	1:B:275:TRP:N	2.84	0.43
1:A:88:ILE:HB	1:A:94:LYS:CE	2.48	0.43
1:A:424:LEU:HD12	1:A:424:LEU:HA	1.89	0.43
1:A:461:TRP:HB3	1:A:465:LYS:HE2	2.00	0.43
1:B:245:ARG:NH2	1:B:245:ARG:CG	2.81	0.43
2:E:337:VAL:CG2	2:E:389:VAL:HG12	2.49	0.43
1:A:68:LYS:HB2	1:A:68:LYS:HE3	1.69	0.43
1:B:457:GLU:CG	1:B:512:PHE:HB3	2.48	0.43
1:A:290:ASN:HB3	1:A:292:ASP:HB3	2.01	0.42
1:B:110:GLU:OE2	1:B:110:GLU:HA	2.19	0.42
1:A:226:VAL:O	1:A:229:THR:HG22	2.19	0.42
1:A:514:ARG:CG	1:A:515:TYR:N	2.81	0.42
2:F:417:MET:CE	2:F:417:MET:HA	2.49	0.42
1:B:520:LEU:HD22	1:B:579:MET:HE3	1.99	0.42
1:B:93:VAL:HG23	1:B:94:LYS:N	2.34	0.42
2:F:389:VAL:HA	2:F:481:TYR:CE1	2.55	0.42
1:A:144:LEU:HA	1:A:148:LEU:HB2	2.00	0.42
1:B:524:GLN:HB3	1:B:574:VAL:HG11	2.00	0.42
2:F:386:SER:HA	2:F:496:VAL:O	2.20	0.42
1:A:145:GLU:HA	1:A:146:PRO:HA	1.87	0.42
1:A:196:TYR:CE2	1:A:202:TYR:HD2	2.38	0.42
1:B:168:TRP:CD1	1:B:502:SER:HB3	2.55	0.42
2:E:323:CYS:N	2:E:348:CYS:SG	2.93	0.42
1:A:419:LYS:O	1:A:421:ILE:N	2.44	0.42
1:A:527:GLU:O	1:A:528:ALA:C	2.57	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:440:LEU:O	1:B:440:LEU:HD13	2.20	0.42
2:F:325:PHE:C	2:F:327:GLU:N	2.73	0.42
1:B:410:LEU:HA	1:B:410:LEU:HD12	1.80	0.41
1:B:581:VAL:HG12	1:B:582:ARG:HH11	1.85	0.41
2:E:442:PHE:CD2	2:E:443:LEU:HG	2.55	0.41
1:A:89:GLN:HB3	1:A:89:GLN:HE21	1.66	0.41
1:B:50:TYR:CE1	1:B:59:VAL:HG23	2.55	0.41
1:B:324:THR:O	1:B:325:GLN:C	2.58	0.41
1:B:457:GLU:HG3	1:B:513:ILE:N	2.35	0.41
1:B:526:GLN:HG3	1:B:539:LEU:HD11	2.02	0.41
1:A:493:HIS:HD2	1:A:499:ASP:OD2	2.03	0.41
1:B:177:ARG:HB3	1:B:178:PRO:HD3	2.01	0.41
1:B:31:LYS:O	1:B:35:GLU:HB2	2.20	0.41
1:B:389:PRO:HG2	1:B:392:LEU:HB2	2.01	0.41
2:F:459:PRO:HA	2:F:477:PRO:HD3	2.02	0.41
1:A:505:HIS:CD2	1:A:505:HIS:H	2.38	0.41
1:A:545:SER:C	1:A:547:SER:H	2.24	0.41
1:B:213:ASP:C	1:B:215:TYR:H	2.24	0.41
2:E:483:PHE:CD1	2:E:493:PRO:HB3	2.56	0.41
1:A:557:MET:HB2	1:A:557:MET:HE3	1.93	0.41
2:E:425:THR:HG21	2:E:495:ARG:HG3	2.01	0.41
2:F:328:VAL:O	2:F:331:ALA:HB3	2.21	0.41
1:B:181:GLU:O	1:B:184:VAL:HG22	2.21	0.41
1:B:288:LYS:HB3	1:B:289:PRO:HD2	2.03	0.41
1:B:83:TYR:HA	1:B:84:PRO:HD3	1.87	0.41
1:A:174:LYS:HG2	1:A:496:THR:O	2.20	0.41
2:F:382:VAL:HG22	2:F:501:PHE:CE2	2.56	0.41
1:A:170:SER:O	1:A:174:LYS:HG3	2.21	0.41
1:B:144:LEU:HB2	1:B:168:TRP:CH2	2.56	0.41
2:E:484:TYR:N	2:E:484:TYR:HD1	2.17	0.41
1:A:425:SER:HA	1:A:426:PRO:HD2	1.89	0.40
2:F:329:PHE:O	2:F:330:ASN:HB2	2.22	0.40
1:A:410:LEU:HD12	1:A:410:LEU:HA	1.84	0.40
1:A:489:GLU:HA	1:A:490:PRO:HD3	1.95	0.40
1:B:174:LYS:HA	1:B:496:THR:O	2.21	0.40
1:B:223:ILE:H	1:B:223:ILE:HG13	1.62	0.40
1:B:270:MET:HB3	1:B:271:TRP:CZ3	2.57	0.40
1:B:521:TYR:O	1:B:522:GLN:C	2.60	0.40
1:B:252:TYR:HD2	1:B:266:LEU:HD13	1.86	0.40
1:A:155:SER:O	1:A:161:ARG:HD2	2.22	0.40
2:F:337:VAL:HB	2:F:409:ASN:HD22	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:165:TRP:HZ2	1:A:478:TRP:HH2	1.70	0.40
1:A:261:CYS:HB2	1:A:488:VAL:HG13	2.03	0.40
1:A:520:LEU:O	1:A:521:TYR:C	2.60	0.40
1:B:187:LYS:O	1:B:190:MET:HB3	2.22	0.40
1:B:392:LEU:HD12	1:B:392:LEU:HA	1.83	0.40
2:E:471:ALA:O	2:E:472:PHE:C	2.60	0.40
2:F:338:TYR:CE1	2:F:455:ILE:HG23	2.57	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	595/603 (99%)	506 (85%)	75 (13%)	14 (2%)	7	27
1	B	595/603 (99%)	516 (87%)	68 (11%)	11 (2%)	10	34
2	E	170/228 (75%)	131 (77%)	28 (16%)	11 (6%)	1	4
2	F	170/228 (75%)	135 (79%)	25 (15%)	10 (6%)	2	6
All	All	1530/1662 (92%)	1288 (84%)	196 (13%)	46 (3%)	5	20

All (46) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	91	LEU
1	A	212	VAL
1	B	91	LEU
1	B	394	ASN
1	B	421	ILE
2	E	402	THR
2	E	415	ASP
2	E	416	PHE

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Mol	Chain	Res	Type
2	E	471	ALA
2	E	472	PHE
2	E	473	ASN
2	F	415	ASP
2	F	472	PHE
2	F	473	ASN
1	A	54	ILE
1	A	289	PRO
1	A	394	ASN
1	A	421	ILE
1	A	504	PHE
1	A	546	ASN
1	B	470	LYS
1	B	509	ASP
2	E	370	SER
2	E	371	ALA
2	F	374	LEU
1	A	420	SER
1	A	614	ALA
1	B	28	PHE
1	B	339	VAL
2	E	463	ASP
2	F	332	THR
2	F	401	GLN
1	A	51	ASN
1	A	64	ASN
1	A	171	GLU
1	B	113	SER
2	E	347	ASN
2	E	401	GLN
2	F	370	SER
2	F	402	THR
1	B	446	ILE
2	F	326	GLY
1	B	89	GLN
1	A	426	PRO
1	B	212	VAL
2	F	470	PRO

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	527/533 (99%)	468 (89%)	59 (11%)	7	21
1	B	527/533 (99%)	467 (89%)	60 (11%)	7	20
2	E	152/202 (75%)	134 (88%)	18 (12%)	6	18
2	F	152/202 (75%)	141 (93%)	11 (7%)	17	43
All	All	1358/1470 (92%)	1210 (89%)	148 (11%)	7	22

All (148) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	THR
1	A	21	ILE
1	A	39	LEU
1	A	47	SER
1	A	53	ASN
1	A	73	LEU
1	A	79	LEU
1	A	87	GLU
1	A	89	GLN
1	A	100	LEU
1	A	110	GLU
1	A	114	LYS
1	A	122	THR
1	A	126	ILE
1	A	142	LEU
1	A	143	LEU
1	A	149	ASN
1	A	156	LEU
1	A	172	VAL
1	A	210	ASN
1	A	212	VAL
1	A	240	LEU
1	A	245	ARG
1	A	278	LEU

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Mol	Chain	Res	Type
1	A	295	ASP
1	A	309	LYS
1	A	317	SER
1	A	333	LEU
1	A	334	THR
1	A	365	THR
1	A	380	GLN
1	A	381	TYR
1	A	385	TYR
1	A	394	ASN
1	A	401	HIS
1	A	410	LEU
1	A	418	LEU
1	A	427	ASP
1	A	429	GLN
1	A	431	ASP
1	A	432	ASN
1	A	439	LEU
1	A	440	LEU
1	A	444	LEU
1	A	455	MET
1	A	460	ARG
1	A	483	GLU
1	A	488	VAL
1	A	493	HIS
1	A	503	LEU
1	A	519	THR
1	A	548	THR
1	A	557	MET
1	A	558	LEU
1	A	559	ARG
1	A	568	LEU
1	A	570	LEU
1	A	578	ASN
1	A	595	LEU
1	B	20	THR
1	B	21	ILE
1	B	27	THR
1	B	29	LEU
1	B	39	LEU
1	B	53	ASN
1	B	55	THR

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Mol	Chain	Res	Type
1	B	79	LEU
1	B	82	MET
1	B	87	GLU
1	B	88	ILE
1	B	100	LEU
1	B	110	GLU
1	B	114	LYS
1	B	129	THR
1	B	142	LEU
1	B	143	LEU
1	B	156	LEU
1	B	172	VAL
1	B	192	ARG
1	B	209	VAL
1	B	216	ASP
1	B	229	THR
1	B	245	ARG
1	B	278	LEU
1	B	287	GLN
1	B	290	ASN
1	B	333	LEU
1	B	334	THR
1	B	381	TYR
1	B	385	TYR
1	B	392	LEU
1	B	394	ASN
1	B	401	HIS
1	B	418	LEU
1	B	429	GLN
1	B	444	LEU
1	B	450	LEU
1	B	455	MET
1	B	462	MET
1	B	482	ARG
1	B	483	GLU
1	B	488	VAL
1	B	491	VAL
1	B	502	SER
1	B	511	SER
1	B	518	ARG
1	B	526	GLN
1	B	529	LEU

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Mol	Chain	Res	Type
1	B	541	LYS
1	B	553	LYS
1	B	557	MET
1	B	560	LEU
1	B	562	LYS
1	B	568	LEU
1	B	573	VAL
1	B	582	ARG
1	B	586	ASN
1	B	595	LEU
1	B	608	THR
2	E	323	CYS
2	E	329	PHE
2	E	334	PHE
2	E	348	CYS
2	E	355	LEU
2	E	356	TYR
2	E	357	ASN
2	E	364	PHE
2	E	369	VAL
2	E	417	MET
2	E	423	TRP
2	E	426	ARG
2	E	427	ASN
2	E	442	PHE
2	E	467	CYS
2	E	468	THR
2	E	484	TYR
2	E	500	SER
2	F	323	CYS
2	F	328	VAL
2	F	348	CYS
2	F	355	LEU
2	F	360	PHE
2	F	364	PHE
2	F	423	TRP
2	F	427	ASN
2	F	442	PHE
2	F	468	THR
2	F	481	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (54) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	24	GLN
1	A	33	ASN
1	A	49	ASN
1	A	51	ASN
1	A	53	ASN
1	A	63	ASN
1	A	81	GLN
1	A	89	GLN
1	A	90	ASN
1	A	96	GLN
1	A	149	ASN
1	A	194	ASN
1	A	300	GLN
1	A	330	ASN
1	A	394	ASN
1	A	432	ASN
1	A	493	HIS
1	A	505	HIS
1	A	508	ASN
1	A	522	GLN
1	A	524	GLN
1	A	540	HIS
1	A	578	ASN
1	A	586	ASN
1	A	599	ASN
1	B	33	ASN
1	B	49	ASN
1	B	51	ASN
1	B	53	ASN
1	B	58	ASN
1	B	61	ASN
1	B	96	GLN
1	B	300	GLN
1	B	330	ASN
1	B	373	HIS
1	B	394	ASN
1	B	493	HIS
1	B	505	HIS
1	B	508	ASN
1	B	522	GLN
1	B	524	GLN
1	B	526	GLN
1	B	531	GLN

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Mol	Chain	Res	Type
1	B	552	GLN
1	B	556	ASN
1	B	572	ASN
1	B	580	ASN
1	B	599	ASN
2	E	409	ASN
2	E	473	ASN
2	F	396	GLN
2	F	409	ASN
2	F	437	ASN
2	F	473	ASN

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 4 ligands modelled in this entry, 4 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, 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	597/603 (99%)	0.21	15 (2%) 58 53	39, 70, 116, 136	0
1	B	597/603 (99%)	0.44	35 (5%) 23 18	38, 73, 119, 138	0
2	E	174/228 (76%)	0.69	22 (12%) 4 3	64, 86, 128, 137	0
2	F	174/228 (76%)	0.59	25 (14%) 3 2	64, 88, 129, 138	0
All	All	1542/1662 (92%)	0.40	97 (6%) 21 16	38, 75, 124, 138	0

All (97) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	501	PHE	6.3
1	B	136	ASP	6.2
2	F	442	PHE	6.0
1	B	615	ASP	5.7
2	F	443	LEU	5.4
2	E	355	LEU	5.2
2	E	352	TYR	4.9
1	B	473	TRP	4.8
2	F	364	PHE	4.8
2	E	421	LEU	4.8
2	E	382	VAL	4.3
2	E	357	ASN	4.3
2	E	472	PHE	4.1
1	A	86	GLN	4.1
2	E	364	PHE	4.0
2	F	354	VAL	3.9
1	B	339	VAL	3.8
2	F	470	PRO	3.6
2	E	358	SER	3.5
1	A	106	SER	3.4
2	F	418	GLY	3.4

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Mol	Chain	Res	Type	RSRZ
2	E	499	LEU	3.4
2	E	500	SER	3.4
2	F	423	TRP	3.4
1	B	135	PRO	3.3
2	F	365	LYS	3.3
2	E	410	TYR	3.2
1	B	84	PRO	3.2
1	B	72	PHE	3.1
2	F	419	CYS	3.1
1	B	130	GLY	3.0
2	E	443	LEU	3.0
2	E	343	LYS	3.0
1	B	560	LEU	3.0
2	F	468	THR	3.0
1	A	85	LEU	2.9
1	B	27	THR	2.9
1	B	79	LEU	2.9
1	A	83	TYR	2.8
1	B	69	TRP	2.8
2	F	325	PHE	2.8
2	F	350	ALA	2.8
2	F	352	TYR	2.8
1	B	171	GLU	2.7
1	A	290	ASN	2.7
1	B	338	ASN	2.7
2	F	356	TYR	2.7
1	A	82	MET	2.7
1	B	26	LYS	2.7
2	F	478	LEU	2.7
1	B	134	ASN	2.6
1	A	298	VAL	2.6
1	B	140	GLU	2.6
1	A	360	MET	2.6
1	B	614	ALA	2.6
2	E	351	ASP	2.6
2	E	359	THR	2.6
1	B	511	SER	2.6
2	F	421	LEU	2.5
1	A	111	ASP	2.5
2	E	442	PHE	2.5
1	B	139	GLN	2.5
2	F	477	PRO	2.5

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Mol	Chain	Res	Type	RSRZ
2	E	412	LEU	2.4
2	F	361	PHE	2.4
2	E	451	PHE	2.4
1	B	129	THR	2.4
2	F	329	PHE	2.4
1	A	296	ALA	2.4
2	F	357	ASN	2.4
1	B	195	HIS	2.4
1	B	64	ASN	2.3
2	F	358	SER	2.3
2	F	353	SER	2.3
1	B	132	VAL	2.3
1	B	164	ALA	2.3
1	B	147	GLY	2.2
1	B	137	ASN	2.2
1	A	119	ILE	2.2
1	B	131	LYS	2.2
1	B	141	CYS	2.1
1	B	186	LEU	2.1
1	A	614	ALA	2.1
1	A	19	SER	2.1
1	B	97	LEU	2.1
2	F	359	THR	2.1
2	F	367	TYR	2.1
1	B	468	ILE	2.1
2	F	360	PHE	2.1
1	B	23	GLU	2.1
2	E	361	PHE	2.1
1	A	84	PRO	2.0
1	B	19	SER	2.0
2	E	344	LYS	2.0
1	A	108	LEU	2.0
1	B	348	ALA	2.0
2	E	325	PHE	2.0

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

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, 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	LLDF	B-factors(Å ²)	Q<0.9
4	CL	A	902	1/1	0.91	0.48	9.78	92,92,92,92	0
4	CL	B	902	1/1	0.88	0.36	5.50	107,107,107,107	0
3	ZN	A	901	1/1	0.94	0.35	-	87,87,87,87	0
3	ZN	B	901	1/1	0.97	0.50	-	90,90,90,90	0

6.5 Other polymers [i](#)

There are no such residues in this entry.