



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2014 – 03:02 AM GMT

PDB ID : 1N8Z
Title : Crystal structure of extracellular domain of human HER2 complexed with Herceptin Fab
Authors : Cho, H.-S.; Mason, K.; Ramyar, K.X.; Stanley, A.M.; Gabelli, S.B.; Denney Jr., D.W.; Leahy, D.J.
Deposited on : 2002-11-21
Resolution : 2.52 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

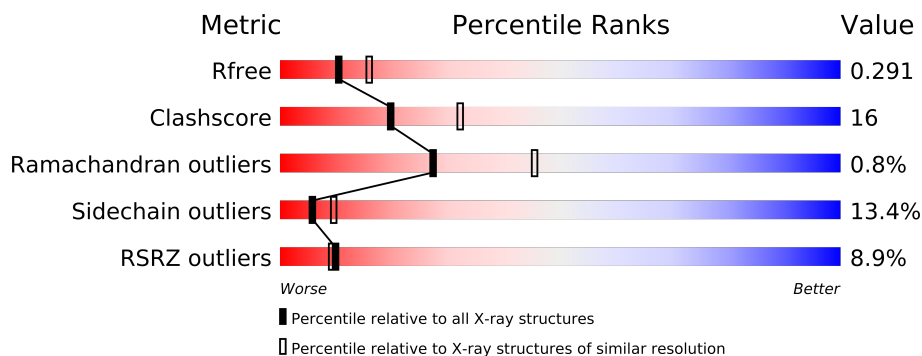
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance




The reported resolution of this entry is 2.52 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}	66092	3240 (2.54-2.50)
Clashscore	79885	4080 (2.54-2.50)
Ramachandran outliers	78287	3990 (2.54-2.50)
Sidechain outliers	78261	3992 (2.54-2.50)
RSRZ outliers	66119	3241 (2.54-2.50)

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 ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	214	
2	B	220	
3	C	607	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
4	NAG	C	766	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 7890 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Herceptin Fab (antibody) - light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	214	Total	C	N	O	S	0	0	0
			1645	1029	276	334	6			

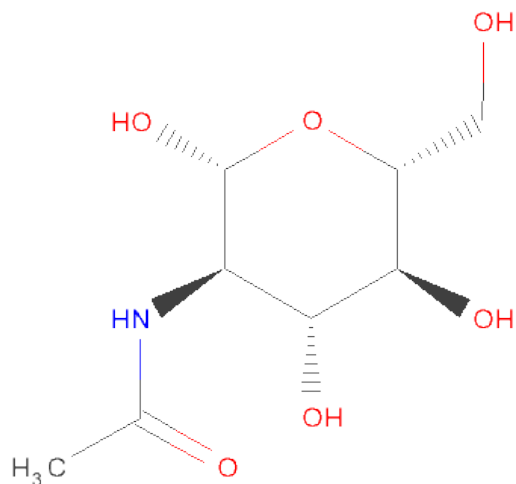
- Molecule 2 is a protein called Herceptin Fab (antibody) - heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	220	Total	C	N	O	S	0	0	0
			1642	1036	276	324	6			

- Molecule 3 is a protein called Receptor protein-tyrosine kinase erbB-2.

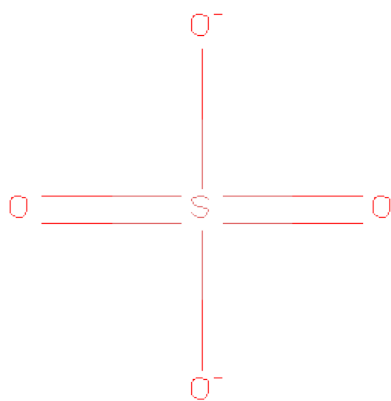
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	581	Total	C	N	O	S	0	0	0
			4491	2796	805	838	52			

- Molecule 4 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: C₈H₁₅NO₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	C	1	Total	C	N	O	0	0
			14	8	1	5		
4	C	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

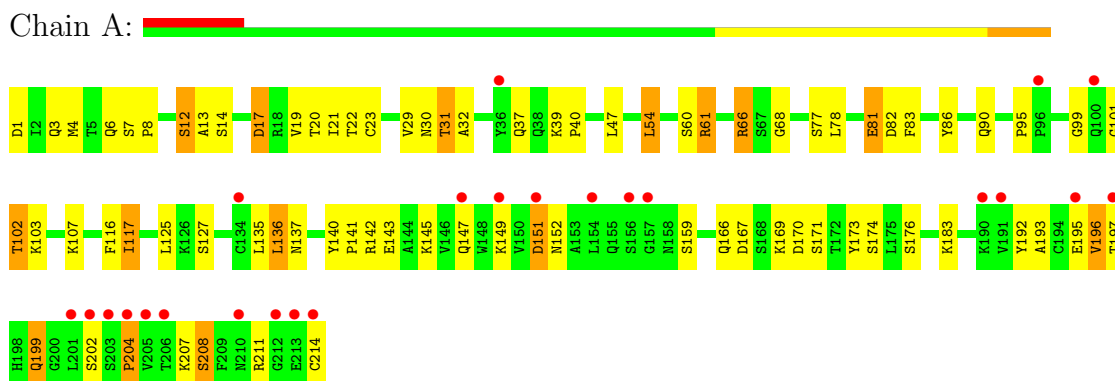
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	19	Total 19	O 19	0	0
6	B	13	Total 13	O 13	0	0
6	C	47	Total 47	O 47	0	0

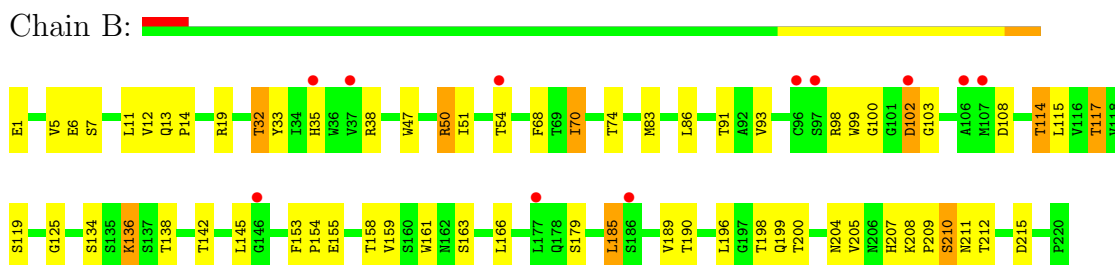
3 Residue-property plots

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.

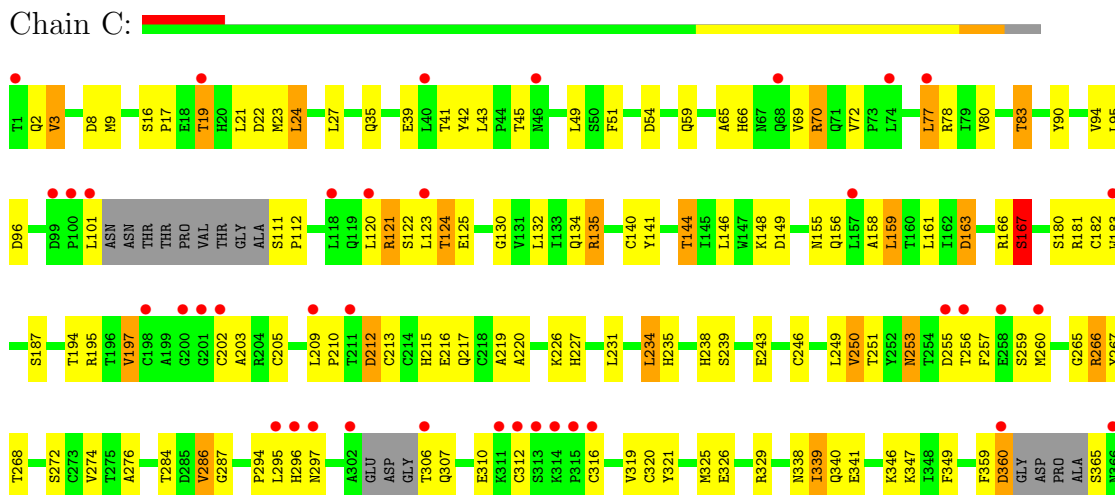
- Molecule 1: Herceptin Fab (antibody) - light chain

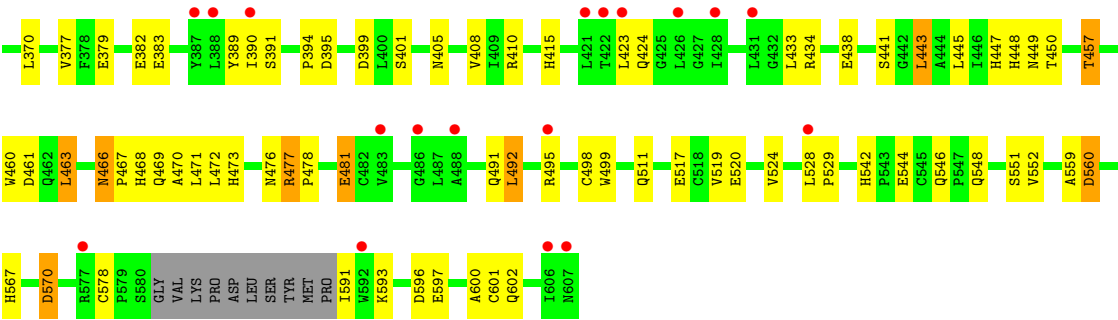


- Molecule 2: Herceptin Fab (antibody) - heavy chain



- Molecule 3: Receptor protein-tyrosine kinase erbB-2





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	66.17Å 109.77Å 175.14Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.52 27.84 – 2.52	Depositor EDS
% Data completeness (in resolution range)	92.9 (20.00-2.52) 89.9 (27.84-2.52)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.26 (at 2.54Å)	Xtriage
Refinement program	REFMAC 5.1.19	Depositor
R, R_{free}	0.222 , 0.284 0.247 , 0.291	Depositor DCC
R_{free} test set	1870 reflections (4.75%)	DCC
Wilson B-factor (Å ²)	43.9	Xtriage
Anisotropy	0.441	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , -0.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 42444 reflections	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	7890	wwPDB-VP
Average B, all atoms (Å ²)	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.38% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

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

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	0.75	0/1682	0.91	3/2288 (0.1%)
2	B	0.72	0/1684	0.91	4/2298 (0.2%)
3	C	0.74	0/4596	0.95	13/6249 (0.2%)
All	All	0.74	0/7962	0.93	20/10835 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
3	C	0	1

There are no bond length outliers.

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	215	ASP	CB-CG-OD2	7.89	125.40	118.30
3	C	560	ASP	CB-CG-OD2	7.29	124.86	118.30
3	C	22	ASP	CB-CG-OD2	6.78	124.40	118.30
1	A	151	ASP	CB-CG-OD2	6.36	124.03	118.30
3	C	477	ARG	NE-CZ-NH2	-6.30	117.15	120.30
3	C	395	ASP	CB-CG-OD2	6.13	123.82	118.30
3	C	54	ASP	CB-CG-OD2	6.12	123.81	118.30
1	A	82	ASP	CB-CG-OD2	5.67	123.41	118.30
2	B	102	ASP	CB-CG-OD2	5.65	123.39	118.30
1	A	167	ASP	CB-CG-OD2	5.58	123.32	118.30
3	C	163	ASP	CB-CG-OD2	5.58	123.32	118.30
3	C	149	ASP	CB-CG-OD2	5.48	123.23	118.30
3	C	443	LEU	CB-CG-CD2	-5.45	101.73	111.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	477	ARG	NE-CZ-NH1	5.18	122.89	120.30
2	B	185	LEU	CA-CB-CG	5.12	127.07	115.30
3	C	8	ASP	CB-CG-OD2	5.10	122.89	118.30
3	C	570	ASP	CB-CG-OD2	5.09	122.89	118.30
3	C	461	ASP	CB-CG-OD2	5.06	122.86	118.30
3	C	212	ASP	CB-CG-OD2	5.06	122.85	118.30
2	B	108	ASP	CB-CG-OD2	5.02	122.82	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	180	SER	Peptide

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1645	0	1589	50	0
2	B	1642	0	1584	45	0
3	C	4491	0	4304	156	0
4	C	28	0	26	3	0
5	C	5	0	0	0	0
6	A	19	0	0	1	0
6	B	13	0	0	0	0
6	C	47	0	0	3	0
All	All	7890	0	7503	246	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 16.

All (246) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:C:457:THR:HG22	3:C:498:CYS:O	1.49	1.10
3:C:266:ARG:HH11	3:C:266:ARG:HG2	1.20	1.03

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:C:124:THR:HG22	3:C:220:ALA:HB1	1.41	1.02
2:B:207:HIS:CD2	2:B:210:SER:HB2	1.98	0.97
3:C:457:THR:CG2	3:C:498:CYS:O	2.15	0.94
1:A:136:LEU:HD21	1:A:196:VAL:HG11	1.52	0.90
3:C:19:THR:CG2	3:C:472:LEU:HB3	2.03	0.88
3:C:542:HIS:HD2	3:C:544:GLU:H	1.21	0.88
1:A:1:ASP:O	1:A:3:GLN:NE2	2.05	0.88
3:C:284:THR:HG22	3:C:286:VAL:H	1.37	0.87
1:A:8:PRO:O	1:A:102:THR:HB	1.75	0.87
3:C:124:THR:CG2	3:C:220:ALA:O	2.23	0.86
3:C:347:LYS:HE3	3:C:383:GLU:OE1	1.76	0.86
2:B:142:THR:CG2	2:B:190:THR:HG22	2.06	0.85
3:C:144:THR:HG23	3:C:181:ARG:HA	1.58	0.85
3:C:578:CYS:HG	3:C:601:CYS:HG	1.21	0.85
3:C:144:THR:CG2	3:C:182:CYS:H	1.90	0.84
3:C:466:ASN:HD22	3:C:468:HIS:H	1.27	0.82
2:B:163:SER:H	2:B:204:ASN:HD21	1.28	0.82
3:C:596:ASP:HB2	3:C:600:ALA:O	1.79	0.82
3:C:166:ARG:C	4:C:766:NAG:H83	2.01	0.81
3:C:96:ASP:OD1	3:C:135:ARG:HD2	1.80	0.81
1:A:12:SER:HB3	1:A:107:LYS:HE3	1.61	0.81
3:C:443:LEU:HD21	3:C:469:GLN:HA	1.64	0.79
3:C:70:ARG:HH11	3:C:70:ARG:HG3	1.47	0.79
3:C:319:VAL:CG1	3:C:320:CYS:N	2.47	0.78
3:C:319:VAL:HG11	3:C:349:PHE:CD1	2.18	0.78
3:C:338:ASN:O	3:C:341:GLU:HB2	1.82	0.78
3:C:19:THR:HG22	3:C:472:LEU:HB3	1.66	0.77
3:C:266:ARG:HH11	3:C:266:ARG:CG	1.97	0.75
3:C:124:THR:HG21	3:C:220:ALA:O	1.85	0.75
3:C:319:VAL:HG12	3:C:320:CYS:N	2.01	0.75
2:B:142:THR:HG23	2:B:190:THR:HG22	1.67	0.75
3:C:141:TYR:O	3:C:144:THR:HB	1.85	0.74
3:C:546:GLN:HE21	3:C:548:GLN:HE22	1.35	0.73
3:C:284:THR:HG22	3:C:286:VAL:N	2.05	0.72
2:B:51:ILE:HB	2:B:70:ILE:CG2	2.20	0.72
3:C:447:HIS:HD2	3:C:448:HIS:CD2	2.09	0.71
1:A:4:MET:HE2	1:A:23:CYS:SG	2.31	0.70
2:B:207:HIS:HD2	2:B:210:SER:HB2	1.54	0.70
3:C:408:VAL:HG12	3:C:438:GLU:HB3	1.75	0.69
2:B:142:THR:CG2	2:B:190:THR:CG2	2.71	0.69
3:C:294:PRO:O	3:C:297:ASN:HB2	1.93	0.69
3:C:449:ASN:H	3:C:476:ASN:HD22	1.41	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:21:ILE:HG23	1:A:102:THR:HG21	1.75	0.68
2:B:51:ILE:HB	2:B:70:ILE:HG23	1.76	0.67
3:C:443:LEU:HD22	3:C:470:ALA:H	1.58	0.67
3:C:424:GLN:HB3	3:C:447:HIS:CE1	2.30	0.67
3:C:542:HIS:CD2	3:C:544:GLU:H	2.09	0.66
1:A:136:LEU:CD2	1:A:196:VAL:HG11	2.25	0.66
3:C:59:GLN:O	3:C:83:THR:HB	1.96	0.66
3:C:217:GLN:HE22	3:C:235:HIS:HD2	1.44	0.64
1:A:14:SER:O	1:A:17:ASP:HB2	1.98	0.63
3:C:399:ASP:OD2	3:C:401:SER:HB3	1.98	0.63
3:C:443:LEU:CD2	3:C:469:GLN:HA	2.28	0.63
3:C:246:CYS:SG	3:C:268:THR:HG22	2.39	0.62
1:A:6:GLN:OE1	1:A:102:THR:HG22	2.00	0.62
2:B:159:VAL:HG22	2:B:205:VAL:HG22	1.81	0.62
2:B:32:THR:HG22	2:B:33:TYR:H	1.65	0.61
3:C:41:THR:HA	3:C:65:ALA:O	2.01	0.61
3:C:319:VAL:CG1	3:C:320:CYS:H	2.14	0.61
3:C:447:HIS:CD2	3:C:448:HIS:HD2	2.20	0.60
1:A:117:ILE:HG22	2:B:136:LYS:HB3	1.83	0.59
2:B:207:HIS:CD2	2:B:210:SER:CB	2.82	0.59
3:C:319:VAL:CG1	3:C:349:PHE:CD1	2.85	0.59
1:A:30:ASN:ND2	1:A:31:THR:HB	2.17	0.59
1:A:166:GLN:HE21	1:A:171:SER:HB3	1.66	0.58
3:C:319:VAL:HG13	3:C:320:CYS:H	1.68	0.58
3:C:542:HIS:CE1	3:C:559:ALA:HB2	2.38	0.58
3:C:389:TYR:CE1	3:C:415:HIS:CE1	2.91	0.58
3:C:443:LEU:CD2	3:C:470:ALA:H	2.16	0.58
3:C:360:ASP:OD1	3:C:360:ASP:N	2.35	0.58
3:C:542:HIS:HD2	3:C:544:GLU:N	1.99	0.58
1:A:116:PHE:HD2	1:A:135:LEU:HD23	1.67	0.58
3:C:447:HIS:CD2	3:C:448:HIS:CD2	2.92	0.58
3:C:326:GLU:O	3:C:329:ARG:HG2	2.04	0.57
3:C:144:THR:HG21	3:C:182:CYS:H	1.68	0.57
1:A:37:GLN:HB2	1:A:47:LEU:HD11	1.85	0.57
3:C:570:ASP:OD2	3:C:593:LYS:NZ	2.35	0.57
3:C:253:ASN:ND2	3:C:256:THR:H	2.03	0.57
1:A:21:ILE:CG2	1:A:102:THR:HG21	2.34	0.57
3:C:9:MET:HG2	3:C:39:GLU:OE1	2.05	0.57
2:B:98:ARG:NE	2:B:100:GLY:HA3	2.20	0.56
3:C:544:GLU:OE1	3:C:567:HIS:HD2	1.87	0.56
2:B:99:TRP:O	2:B:100:GLY:C	2.42	0.56
1:A:4:MET:CE	1:A:23:CYS:SG	2.92	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:197:THR:HG23	1:A:204:PRO:HG3	1.87	0.56
1:A:116:PHE:CD2	1:A:135:LEU:HD23	2.41	0.56
1:A:12:SER:HB3	1:A:107:LYS:CE	2.34	0.56
3:C:19:THR:HG21	3:C:445:LEU:CD1	2.36	0.56
3:C:478:PRO:O	3:C:481:GLU:HB2	2.06	0.56
3:C:447:HIS:HD2	3:C:448:HIS:HD2	1.49	0.55
3:C:528:LEU:HB2	3:C:529:PRO:HD3	1.89	0.55
1:A:95:PRO:HB3	2:B:47:TRP:CZ3	2.42	0.55
1:A:136:LEU:HD12	1:A:136:LEU:N	2.22	0.55
3:C:274:VAL:HG13	3:C:276:ALA:O	2.06	0.55
3:C:210:PRO:O	3:C:213:CYS:HB2	2.07	0.54
2:B:207:HIS:HD2	2:B:210:SER:CB	2.19	0.54
2:B:12:VAL:HG12	2:B:13:GLN:O	2.08	0.54
1:A:192:TYR:O	1:A:208:SER:HA	2.08	0.54
3:C:391:SER:HB2	6:C:1031:HOH:O	2.07	0.54
2:B:33:TYR:CD2	2:B:50:ARG:HD2	2.43	0.54
3:C:253:ASN:HD22	3:C:255:ASP:H	1.56	0.54
1:A:6:GLN:HE21	1:A:99:GLY:HA3	1.73	0.53
3:C:434:ARG:HA	3:C:499:TRP:CD1	2.43	0.53
3:C:408:VAL:O	3:C:408:VAL:HG23	2.09	0.53
2:B:11:LEU:HD11	2:B:153:PHE:HE1	1.75	0.52
3:C:266:ARG:NH1	3:C:266:ARG:HG2	2.00	0.52
3:C:578:CYS:HG	3:C:601:CYS:CB	2.22	0.52
3:C:215:HIS:HD2	3:C:217:GLN:H	1.58	0.52
3:C:319:VAL:HG11	3:C:349:PHE:CE1	2.44	0.52
3:C:125:GLU:OE1	3:C:219:ALA:O	2.26	0.52
3:C:466:ASN:ND2	3:C:468:HIS:H	2.03	0.52
1:A:22:THR:HG22	1:A:23:CYS:N	2.24	0.52
1:A:19:VAL:HG21	1:A:78:LEU:HD13	1.92	0.52
2:B:210:SER:HB3	2:B:212:THR:OG1	2.09	0.51
2:B:142:THR:HG21	2:B:190:THR:CG2	2.40	0.51
1:A:193:ALA:HA	1:A:208:SER:HB2	1.93	0.51
3:C:135:ARG:CG	3:C:135:ARG:HH11	2.24	0.51
1:A:4:MET:SD	1:A:90:GLN:HB3	2.51	0.51
3:C:19:THR:HG22	3:C:472:LEU:HD13	1.92	0.51
3:C:321:TYR:CE2	3:C:326:GLU:HG3	2.44	0.51
1:A:13:ALA:HB3	1:A:78:LEU:HD22	1.92	0.51
3:C:194:THR:HG23	3:C:205:CYS:O	2.10	0.51
3:C:49:LEU:HD13	3:C:72:VAL:HG12	1.93	0.51
2:B:98:ARG:CZ	2:B:100:GLY:HA3	2.41	0.50
3:C:24:LEU:CD2	3:C:43:LEU:HD21	2.42	0.50
3:C:209:LEU:O	3:C:212:ASP:HB2	2.12	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:86:TYR:O	1:A:101:GLY:HA2	2.12	0.50
3:C:286:VAL:HG13	3:C:286:VAL:O	2.12	0.50
3:C:249:LEU:HD11	3:C:267:TYR:CE2	2.46	0.50
3:C:466:ASN:HD22	3:C:468:HIS:N	2.05	0.50
1:A:83:PHE:CE1	1:A:166:GLN:HB3	2.46	0.50
1:A:125:LEU:O	1:A:183:LYS:HD2	2.11	0.50
3:C:266:ARG:NH1	3:C:266:ARG:CG	2.63	0.49
2:B:33:TYR:HD2	2:B:50:ARG:HD2	1.77	0.49
3:C:253:ASN:ND2	3:C:255:ASP:H	2.11	0.49
1:A:30:ASN:HD21	3:C:602:GLN:HE22	1.60	0.49
3:C:267:TYR:HA	3:C:287:GLY:O	2.13	0.49
3:C:195:ARG:HG3	3:C:203:ALA:O	2.12	0.49
3:C:466:ASN:ND2	3:C:468:HIS:HB2	2.27	0.49
3:C:24:LEU:HD23	3:C:43:LEU:HD21	1.93	0.49
2:B:91:THR:HG23	2:B:117:THR:HA	1.95	0.48
3:C:156:GLN:C	3:C:158:ALA:H	2.15	0.48
3:C:130:GLY:HA3	3:C:159:LEU:O	2.14	0.48
2:B:98:ARG:NE	2:B:100:GLY:CA	2.76	0.48
1:A:39:LYS:NZ	1:A:81:GLU:O	2.35	0.48
3:C:96:ASP:CG	3:C:135:ARG:HD2	2.33	0.48
3:C:94:VAL:O	3:C:95:LEU:HD23	2.13	0.48
2:B:134:SER:O	2:B:138:THR:HG23	2.13	0.48
3:C:466:ASN:HD21	3:C:468:HIS:HB2	1.79	0.47
1:A:30:ASN:HD22	1:A:31:THR:HB	1.79	0.47
1:A:140:TYR:CG	1:A:141:PRO:HA	2.49	0.47
3:C:70:ARG:NH1	3:C:70:ARG:HG3	2.21	0.47
3:C:42:TYR:HA	3:C:66:HIS:O	2.15	0.47
3:C:600:ALA:O	3:C:602:GLN:NE2	2.47	0.47
2:B:154:PRO:O	2:B:207:HIS:HE1	1.98	0.47
1:A:61:ARG:HB3	6:A:228:HOH:O	2.15	0.47
3:C:382:GLU:HA	3:C:405:ASN:O	2.15	0.47
3:C:473:HIS:ND1	3:C:473:HIS:O	2.48	0.47
3:C:460:TRP:CE3	3:C:463:LEU:HD23	2.50	0.47
3:C:238:HIS:HD2	3:C:243:GLU:OE2	1.98	0.47
3:C:424:GLN:HA	3:C:447:HIS:O	2.15	0.46
3:C:253:ASN:HB3	3:C:257:PHE:H	1.80	0.46
2:B:83:MET:HB3	2:B:86:LEU:HD21	1.98	0.46
3:C:524:VAL:HG13	3:C:552:VAL:HG22	1.96	0.46
3:C:466:ASN:HB2	3:C:467:PRO:HD2	1.96	0.46
3:C:215:HIS:HD2	3:C:217:GLN:HB2	1.81	0.46
1:A:61:ARG:NH2	1:A:81:GLU:OE1	2.49	0.46
2:B:51:ILE:HB	2:B:70:ILE:HG21	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:208:SER:O	2:B:136:LYS:HD2	2.15	0.46
1:A:199:GLN:H	1:A:199:GLN:HG2	1.34	0.46
3:C:90:TYR:CD2	3:C:132:LEU:HB2	2.51	0.46
3:C:250:VAL:HG21	3:C:259:SER:HB3	1.98	0.46
3:C:219:ALA:HB2	3:C:234:LEU:HA	1.97	0.45
3:C:78:ARG:HD3	3:C:231:LEU:HB3	1.98	0.45
3:C:511:GLN:HB2	3:C:519:VAL:O	2.16	0.45
3:C:155:ASN:O	3:C:158:ALA:HB2	2.16	0.45
3:C:265:GLY:O	3:C:266:ARG:HG2	2.16	0.45
2:B:115:LEU:CD2	2:B:155:GLU:HB3	2.47	0.45
3:C:491:GLN:OE1	3:C:491:GLN:HA	2.17	0.45
3:C:124:THR:CG2	3:C:220:ALA:HB1	2.30	0.45
3:C:197:VAL:HG13	3:C:197:VAL:O	2.17	0.45
2:B:98:ARG:NH2	2:B:100:GLY:HA3	2.32	0.45
3:C:359:PHE:CZ	3:C:394:PRO:HD3	2.51	0.45
3:C:424:GLN:CB	3:C:447:HIS:CE1	3.00	0.44
1:A:54:LEU:HD11	1:A:60:SER:HA	1.99	0.44
3:C:167:SER:N	4:C:766:NAG:H83	2.31	0.44
1:A:29:VAL:O	1:A:29:VAL:CG1	2.65	0.44
2:B:68:PHE:N	2:B:68:PHE:CD1	2.85	0.44
3:C:249:LEU:HD11	3:C:267:TYR:CZ	2.52	0.44
3:C:238:HIS:CD2	3:C:243:GLU:OE2	2.71	0.44
2:B:6:GLU:HB3	2:B:114:THR:OG1	2.18	0.44
3:C:166:ARG:O	4:C:766:NAG:H83	2.17	0.43
3:C:70:ARG:HG3	6:C:1019:HOH:O	2.17	0.43
3:C:3:VAL:HG11	3:C:35:GLN:HE21	1.83	0.43
2:B:13:GLN:HG3	2:B:14:PRO:HD2	2.00	0.43
2:B:12:VAL:HG11	2:B:86:LEU:HD12	2.00	0.43
1:A:54:LEU:HA	1:A:54:LEU:HD23	1.65	0.43
3:C:96:ASP:HA	3:C:135:ARG:O	2.18	0.43
3:C:215:HIS:CD2	3:C:217:GLN:HB2	2.54	0.43
2:B:103:GLY:O	3:C:593:LYS:NZ	2.42	0.43
3:C:560:ASP:OD1	3:C:560:ASP:C	2.56	0.43
3:C:140:CYS:O	3:C:141:TYR:HB2	2.19	0.43
3:C:274:VAL:CG1	3:C:276:ALA:O	2.66	0.43
3:C:520:GLU:HB3	6:C:1047:HOH:O	2.19	0.43
2:B:161:TRP:HB3	2:B:166:LEU:HD23	1.99	0.43
3:C:256:THR:O	3:C:257:PHE:HB2	2.18	0.43
3:C:339:ILE:HG23	3:C:340:GLN:HG2	2.00	0.42
3:C:390:ILE:HB	3:C:423:LEU:HD23	2.01	0.42
3:C:121:ARG:HA	3:C:183:TRP:CD1	2.53	0.42
3:C:383:GLU:HG3	3:C:408:VAL:HG23	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:142:ARG:HB2	1:A:173:TYR:CE2	2.55	0.42
2:B:145:LEU:HD12	2:B:189:VAL:HG12	2.02	0.42
2:B:207:HIS:CE1	2:B:209:PRO:HG2	2.54	0.42
3:C:450:THR:O	3:C:477:ARG:HG3	2.20	0.42
3:C:528:LEU:CB	3:C:529:PRO:HD3	2.50	0.42
1:A:66:ARG:HD2	1:A:68:GLY:O	2.20	0.42
1:A:81:GLU:H	1:A:81:GLU:HG3	1.58	0.41
1:A:7:SER:HB2	1:A:8:PRO:HA	2.01	0.41
3:C:78:ARG:CZ	3:C:122:SER:HB3	2.50	0.41
3:C:492:LEU:HD11	3:C:520:GLU:OE1	2.21	0.41
3:C:16:SER:HA	3:C:17:PRO:HD3	1.73	0.41
2:B:125:GLY:CA	2:B:210:SER:OG	2.68	0.41
3:C:134:GLN:HA	3:C:163:ASP:HB3	2.02	0.41
3:C:286:VAL:CG1	3:C:286:VAL:O	2.69	0.41
3:C:135:ARG:CG	3:C:135:ARG:NH1	2.83	0.41
3:C:524:VAL:CG1	3:C:552:VAL:HG22	2.51	0.41
3:C:77:LEU:HD13	3:C:123:LEU:HD13	2.02	0.41
3:C:16:SER:OG	3:C:19:THR:OG1	2.36	0.41
3:C:155:ASN:O	3:C:158:ALA:CB	2.69	0.41
2:B:33:TYR:HB3	2:B:50:ARG:HD2	2.02	0.41
2:B:14:PRO:HD3	2:B:119:SER:C	2.41	0.41
3:C:120:LEU:HB2	3:C:183:TRP:CZ3	2.56	0.41
1:A:6:GLN:NE2	1:A:101:GLY:H	2.18	0.41
1:A:107:LYS:HA	1:A:140:TYR:OH	2.20	0.41
3:C:433:LEU:HB2	3:C:499:TRP:CZ3	2.56	0.41
2:B:35:HIS:CE1	2:B:50:ARG:HD3	2.55	0.41
1:A:29:VAL:HG12	1:A:29:VAL:O	2.19	0.41
3:C:477:ARG:HA	3:C:478:PRO:HD3	1.95	0.40
2:B:38:ARG:HA	2:B:93:VAL:O	2.21	0.40
3:C:111:SER:HA	3:C:112:PRO:HA	1.86	0.40
1:A:170:ASP:C	1:A:170:ASP:OD1	2.59	0.40
3:C:410:ARG:NH1	3:C:410:ARG:HG2	2.36	0.40
3:C:23:MET:HG2	3:C:443:LEU:HD12	2.02	0.40
3:C:231:LEU:HD23	3:C:231:LEU:HA	1.82	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	212/214 (99%)	190 (90%)	17 (8%)	5 (2%)	9	13
2	B	218/220 (99%)	210 (96%)	8 (4%)	0	100	100
3	C	571/607 (94%)	518 (91%)	50 (9%)	3 (0%)	38	60
All	All	1001/1041 (96%)	918 (92%)	75 (8%)	8 (1%)	27	45

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	151	ASP
3	C	167	SER
1	A	32	ALA
1	A	152	ASN
3	C	51	PHE
3	C	187	SER
1	A	40	PRO
1	A	204	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	188/189 (100%)	157 (84%)	31 (16%)	3	5
2	B	179/181 (99%)	156 (87%)	23 (13%)	6	11
3	C	503/523 (96%)	440 (88%)	63 (12%)	7	11
All	All	870/893 (97%)	753 (87%)	117 (13%)	6	9

All (117) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	SER
1	A	17	ASP
1	A	20	THR
1	A	31	THR
1	A	54	LEU
1	A	61	ARG
1	A	66	ARG
1	A	77	SER
1	A	81	GLU
1	A	102	THR
1	A	103	LYS
1	A	117	ILE
1	A	127	SER
1	A	136	LEU
1	A	137	ASN
1	A	143	GLU
1	A	145	LYS
1	A	147	GLN
1	A	149	LYS
1	A	159	SER
1	A	169	LYS
1	A	174	SER
1	A	176	SER
1	A	195	GLU
1	A	196	VAL
1	A	199	GLN
1	A	202	SER
1	A	207	LYS
1	A	208	SER
1	A	211	ARG
1	A	214	CYS
2	B	1	GLU
2	B	5	VAL
2	B	7	SER
2	B	19	ARG
2	B	32	THR
2	B	50	ARG
2	B	54	THR
2	B	70	ILE
2	B	74	THR
2	B	102	ASP
2	B	114	THR
2	B	117	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	136	LYS
2	B	158	THR
2	B	179	SER
2	B	185	LEU
2	B	196	LEU
2	B	198	THR
2	B	199	GLN
2	B	200	THR
2	B	208	LYS
2	B	210	SER
2	B	211	ASN
3	C	2	GLN
3	C	3	VAL
3	C	19	THR
3	C	21	LEU
3	C	24	LEU
3	C	27	LEU
3	C	45	THR
3	C	69	VAL
3	C	70	ARG
3	C	77	LEU
3	C	80	VAL
3	C	83	THR
3	C	101	LEU
3	C	121	ARG
3	C	124	THR
3	C	135	ARG
3	C	144	THR
3	C	146	LEU
3	C	148	LYS
3	C	159	LEU
3	C	161	LEU
3	C	167	SER
3	C	197	VAL
3	C	202	CYS
3	C	216	GLU
3	C	226	LYS
3	C	227	HIS
3	C	234	LEU
3	C	239	SER
3	C	250	VAL
3	C	251	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	C	253	ASN
3	C	260	MET
3	C	266	ARG
3	C	272	SER
3	C	286	VAL
3	C	295	LEU
3	C	296	HIS
3	C	306	THR
3	C	307	GLN
3	C	310	GLU
3	C	312	CYS
3	C	316	CYS
3	C	325	MET
3	C	339	ILE
3	C	346	LYS
3	C	360	ASP
3	C	365	SER
3	C	370	LEU
3	C	377	VAL
3	C	379	GLU
3	C	441	SER
3	C	457	THR
3	C	463	LEU
3	C	466	ASN
3	C	471	LEU
3	C	481	GLU
3	C	492	LEU
3	C	495	ARG
3	C	517	GLU
3	C	551	SER
3	C	591	ILE
3	C	597	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6	GLN
1	A	30	ASN
1	A	89	GLN
1	A	91	HIS
1	A	137	ASN
1	A	138	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	204	ASN
2	B	207	HIS
2	B	211	ASN
3	C	2	GLN
3	C	26	HIS
3	C	66	HIS
3	C	156	GLN
3	C	215	HIS
3	C	217	GLN
3	C	227	HIS
3	C	235	HIS
3	C	238	HIS
3	C	245	HIS
3	C	253	ASN
3	C	296	HIS
3	C	307	GLN
3	C	405	ASN
3	C	415	HIS
3	C	424	GLN
3	C	447	HIS
3	C	448	HIS
3	C	456	HIS
3	C	466	ASN
3	C	476	ASN
3	C	526	GLN
3	C	542	HIS
3	C	546	GLN
3	C	567	HIS

5.3.3 RNA ⓘ

There are no RNA chains 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

3 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	SO4	C	1001	-	4,4,4	0.31	0	6,6,6	0.66	0
4	NAG	C	738	3	12,14,15	0.68	0	15,19,21	1.57	3 (20%)
4	NAG	C	766	3	12,14,15	0.89	0	15,19,21	2.61	7 (46%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	SO4	C	1001	-	-	0/0/0/0	0/0/0/0
4	NAG	C	738	3	-	0/6/23/26	0/1/1/1
4	NAG	C	766	3	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	766	NAG	O5-C5-C6	6.72	114.03	106.98
4	C	738	NAG	C3-C2-N2	-3.88	105.86	111.76
4	C	766	NAG	C3-C2-N2	-3.56	106.33	111.76
4	C	766	NAG	O3-C3-C4	3.23	117.60	110.35
4	C	738	NAG	C3-C4-C5	3.16	115.84	110.20
4	C	766	NAG	O5-C5-C4	-2.82	107.07	110.65
4	C	766	NAG	C6-C5-C4	2.77	119.69	113.00
4	C	766	NAG	C2-N2-C7	-2.56	118.78	123.09
4	C	766	NAG	C3-C4-C5	-2.18	106.30	110.20
4	C	738	NAG	O4-C4-C3	-2.05	105.76	110.35

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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	214/214 (100%)	0.68	24 (11%) 6 6	7, 16, 24, 33	0
2	B	220/220 (100%)	0.43	11 (5%) 28 29	8, 16, 24, 35	0
3	C	581/607 (95%)	0.61	56 (9%) 8 8	2, 16, 25, 38	0
All	All	1015/1041 (97%)	0.59	91 (8%) 10 9	2, 16, 24, 38	0

All (91) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	214	CYS	6.9
3	C	201	GLY	6.0
3	C	315	PRO	4.9
1	A	212	GLY	4.8
3	C	607	ASN	4.7
3	C	592	TRP	4.5
3	C	606	ILE	4.5
3	C	388	LEU	4.4
3	C	390	ILE	4.3
3	C	101	LEU	4.1
3	C	316	CYS	4.1
3	C	120	LEU	3.9
3	C	295	LEU	3.8
3	C	423	LEU	3.8
1	A	154	LEU	3.6
3	C	313	SER	3.6
3	C	306	THR	3.5
3	C	422	THR	3.5
3	C	260	MET	3.4
3	C	157	LEU	3.4
3	C	421	LEU	3.4
3	C	314	LYS	3.4
1	A	213	GLU	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	C	1	THR	3.3
1	A	151	ASP	3.2
3	C	296	HIS	3.2
3	C	312	CYS	3.1
3	C	118	LEU	3.1
3	C	528	LEU	3.0
3	C	100	PRO	3.0
3	C	495	ARG	3.0
3	C	123	LEU	3.0
1	A	191	VAL	3.0
1	A	201	LEU	2.9
1	A	202	SER	2.9
3	C	311	LYS	2.8
3	C	483	VAL	2.8
2	B	107	MET	2.8
1	A	197	THR	2.7
3	C	183	TRP	2.7
3	C	297	ASN	2.7
3	C	258	GLU	2.7
2	B	97	SER	2.7
3	C	77	LEU	2.6
3	C	256	THR	2.6
2	B	96	CYS	2.6
1	A	157	GLY	2.5
3	C	577	ARG	2.5
3	C	360	ASP	2.5
3	C	209	LEU	2.5
1	A	156	SER	2.5
1	A	210	ASN	2.5
3	C	202	CYS	2.4
3	C	19	THR	2.4
3	C	426	LEU	2.4
1	A	36	TYR	2.4
1	A	134	CYS	2.4
1	A	149	LYS	2.4
3	C	255	ASP	2.4
1	A	147	GLN	2.4
2	B	106	ALA	2.4
3	C	200	GLY	2.4
1	A	203	SER	2.3
3	C	431	LEU	2.3
1	A	204	PRO	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	C	488	ALA	2.3
3	C	211	THR	2.3
3	C	387	TYR	2.3
2	B	35	HIS	2.3
3	C	46	ASN	2.3
1	A	96	PRO	2.3
3	C	198	CYS	2.2
1	A	206	THR	2.2
3	C	486	GLY	2.2
3	C	302	ALA	2.2
2	B	37	VAL	2.2
1	A	195	GLU	2.2
2	B	102	ASP	2.2
3	C	99	ASP	2.2
2	B	146	GLY	2.2
3	C	74	LEU	2.1
2	B	54	THR	2.1
3	C	40	LEU	2.1
1	A	100	GLN	2.1
3	C	428	ILE	2.1
2	B	177	LEU	2.1
1	A	190	LYS	2.0
2	B	186	SER	2.0
3	C	68	GLN	2.0
1	A	205	VAL	2.0
3	C	366	ASN	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 ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	NAG	C	766	14/15	0.23	2.44	48,55,58,59	0
5	SO4	C	1001	5/5	0.22	1.34	59,60,61,62	0
4	NAG	C	738	14/15	0.14	0.16	33,43,46,47	0

6.5 Other polymers ⓘ

There are no such residues in this entry.