Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 10:56 AM GMT

PDB ID	:	3NJP
Title	:	The Extracellular and Transmembrane Domain Interfaces in Epidermal Growth Factor Receptor Signaling
Authors	:	Lu, C.; Mi, L.-Z.; Grey, M.J.; Zhu, J.; Graef, E.; Yokoyama, S.; Springer, T.A.
Deposited on	:	2010-06-17
Resolution	:	3.30 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

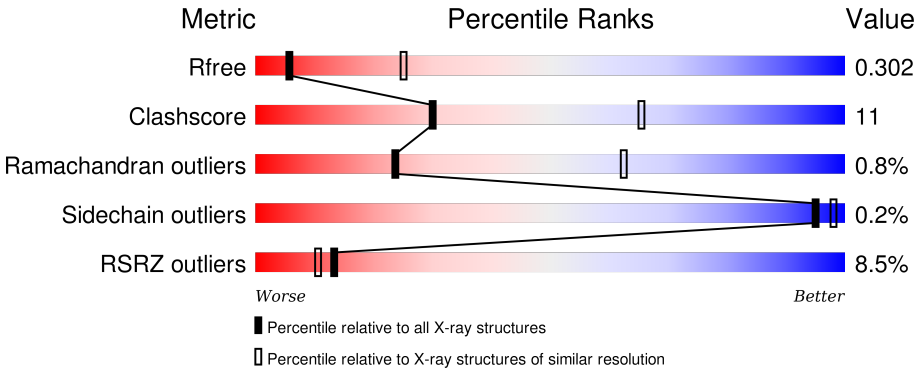
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 3.30 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	2060 (3.40-3.20)
Clashscore	102246	1058 (3.38-3.22)
Ramachandran outliers	100387	1038 (3.38-3.22)
Sidechain outliers	100360	1037 (3.38-3.22)
RSRZ outliers	91569	2070 (3.40-3.20)

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 <=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	614	9% 75% 25%
1	B	614	9% 73% 26%
2	C	47	94% 6%
2	D	47	4% 77% 23%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NAG	A	1172	X	-	-	-
3	NAG	A	1337	X	-	-	-
3	NAG	B	1504	X	-	-	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 10567 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 Epidermal growth factor receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	614	Total	C	N	O	S	0	1	0
			4733	2921	844	908	60			
1	B	614	Total	C	N	O	S	0	1	0
			4730	2919	842	909	60			

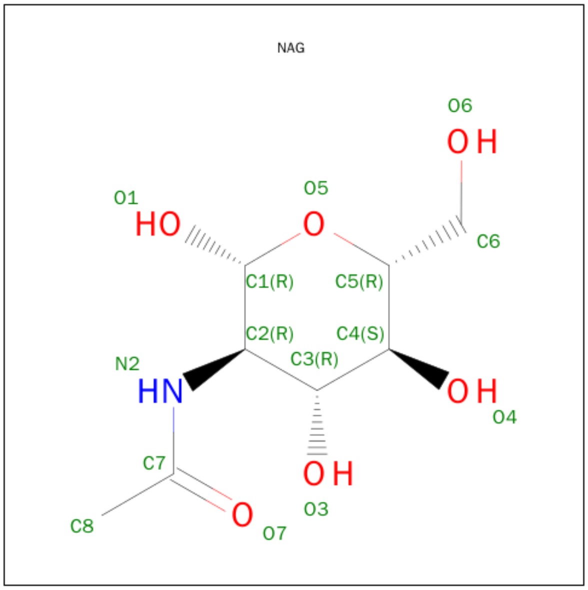
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	516	LYS	ASN	CONFLICT	UNP P00533
B	516	LYS	ASN	CONFLICT	UNP P00533

- Molecule 2 is a protein called Epidermal growth factor.

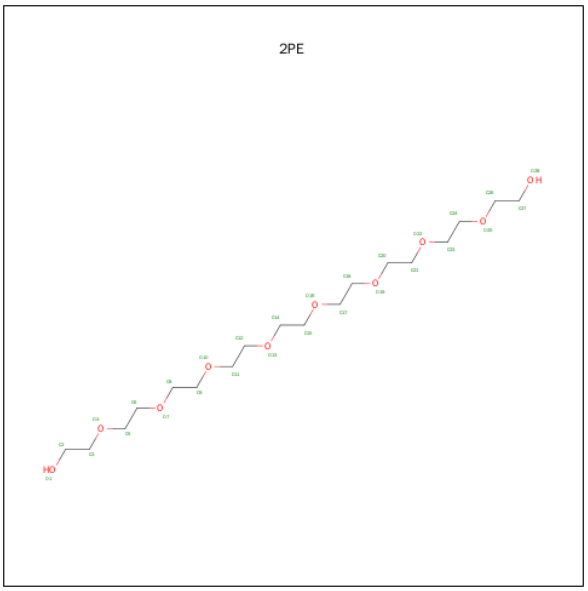
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	47	Total	C	N	O	S	0	0	0
			386	244	63	72	7			
2	D	47	Total	C	N	O	S	0	0	0
			386	244	63	72	7			

- Molecule 3 is polyethyleneglycol (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O 14 8 1 5	0	0
3	A	1	Total C N O 14 8 1 5	0	0
3	A	1	Total C N O 14 8 1 5	0	0
3	A	1	Total C N O 14 8 1 5	0	0
3	A	1	Total C N O 14 8 1 5	0	0
3	A	1	Total C N O 14 8 1 5	0	0
3	A	1	Total C N O 14 8 1 5	0	0
3	A	1	Total C N O 14 8 1 5	0	0
3	B	1	Total C N O 14 8 1 5	0	0
3	B	1	Total C N O 14 8 1 5	0	0
3	B	1	Total C N O 14 8 1 5	0	0
3	B	1	Total C N O 14 8 1 5	0	0

- Molecule 4 is NONAETHYLENE GLYCOL (three-letter code: 2PE) (formula: $C_{18}H_{38}O_{10}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total C O 28 18 10	0	0
4	B	1	Total C O 28 18 10	0	0
4	B	1	Total C O 28 18 10	0	0
4	D	1	Total C O 28 18 10	0	0
4	D	1	Total C O 28 18 10	0	0

- Molecule 5 is water.

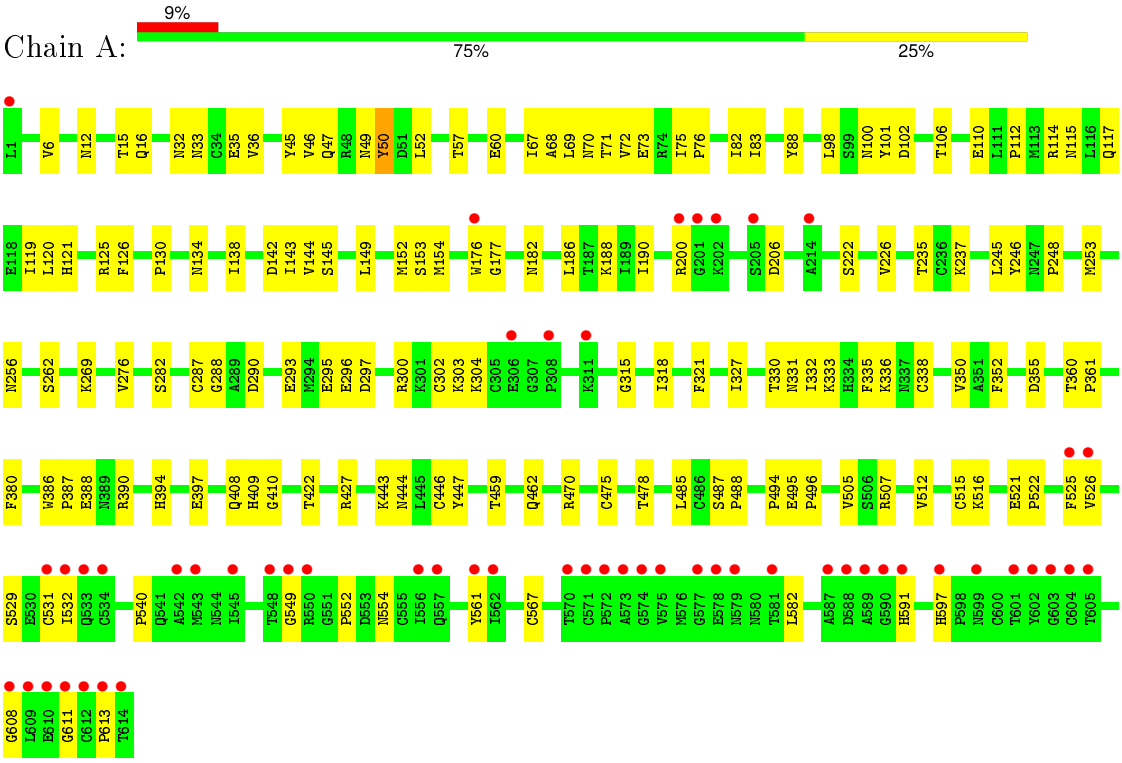
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	13	Total O 13 13	0	0
5	B	5	Total O 5 5	0	0
5	C	5	Total O 5 5	0	0
5	D	1	Total O 1 1	0	0

3 Residue-property plots (i)

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.

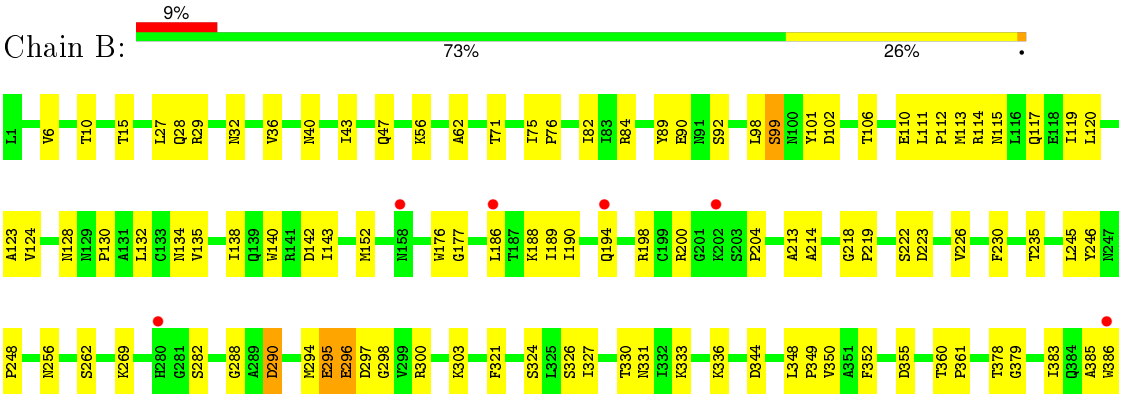
- Molecule 1: Epidermal growth factor receptor

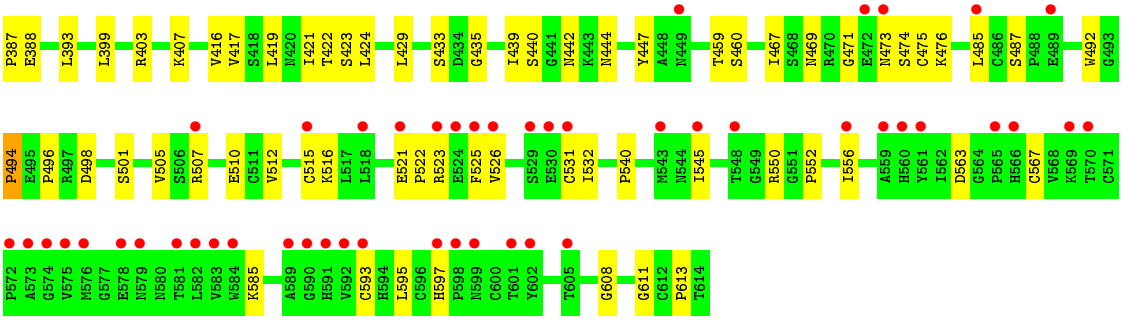
Chain A:



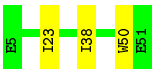
- Molecule 1: Epidermal growth factor receptor

Chain B:

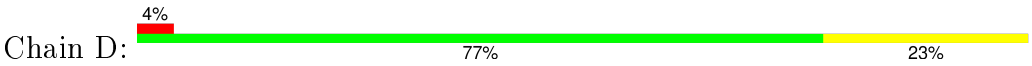


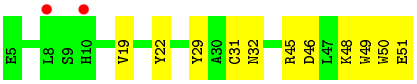


- Molecule 2: Epidermal growth factor



- Molecule 2: Epidermal growth factor





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	220.17Å 220.17Å 113.12Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.49 – 3.30 49.49 – 3.30	Depositor EDS
% Data completeness (in resolution range)	98.2 (49.49-3.30) 98.2 (49.49-3.30)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.76 (at 3.33Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.263 , 0.298 0.263 , 0.302	Depositor DCC
R_{free} test set	2322 reflections (5.24%)	DCC
Wilson B-factor (Å^2)	92.1	Xtriage
Anisotropy	0.127	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 78.9	EDS
Estimated twinning fraction	0.037 for -h,-k,l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.28$	Xtriage
Outliers	0 of 46659 reflections	Xtriage
F_o,F_c correlation	0.86	EDS
Total number of atoms	10567	wwPDB-VP
Average B, all atoms (Å^2)	127.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.15% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 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: 2PE, NAG

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	0.21	0/4828	0.38	0/6528
1	B	0.21	0/4825	0.38	0/6525
2	C	0.22	0/397	0.34	0/536
2	D	0.21	0/397	0.36	0/536
All	All	0.21	0/10447	0.38	0/14125

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	4733	0	4565	106	0
1	B	4730	0	4563	115	0
2	C	386	0	344	2	0
2	D	386	0	344	10	0
3	A	112	0	104	2	0
3	B	56	0	52	3	0
4	B	84	0	114	1	0
4	D	56	0	76	1	0
5	A	13	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	5	0	0	0	0
5	C	5	0	0	0	0
5	D	1	0	0	0	0
All	All	10567	0	10162	230	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 11.

All (230) 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:A:521:GLU:HB2	1:A:522:PRO:HD3	1.51	0.91
2:D:45:ARG:HG2	2:D:45:ARG:HH11	1.35	0.90
1:B:521:GLU:HB3	1:B:522:PRO:HD3	1.57	0.84
1:B:505:VAL:HG23	1:B:512:VAL:HG23	1.62	0.79
1:B:422:THR:HA	1:B:444:ASN:O	1.87	0.74
1:B:194:GLN:HE21	1:B:204:PRO:HB3	1.55	0.72
1:B:222:SER:HB3	1:B:235:THR:HG22	1.72	0.72
1:B:447:TYR:OH	1:B:494:PRO:HG3	1.90	0.71
1:B:523:ARG:NH1	1:B:540:PRO:HB3	2.05	0.71
1:A:46:VAL:HG11	1:A:52:LEU:HD11	1.72	0.70
1:B:597:HIS:HB2	1:B:608:GLY:HA2	1.73	0.69
1:B:349:PRO:HG3	1:B:385:ALA:HB2	1.74	0.69
4:B:616:2PE:H171	4:B:617:2PE:H52	1.75	0.68
2:D:45:ARG:HG2	2:D:45:ARG:NH1	2.09	0.67
1:B:471:GLY:HA3	1:B:475:CYS:SG	2.34	0.67
1:A:149:LEU:HA	1:A:152:MET:HG3	1.77	0.67
1:B:523:ARG:HD2	1:B:540:PRO:HA	1.80	0.63
1:A:222:SER:HB3	1:A:235:THR:HG22	1.81	0.62
1:A:422:THR:HA	1:A:444:ASN:O	1.99	0.62
1:A:321:PHE:CE1	1:A:331:ASN:HB2	2.34	0.62
1:A:388:GLU:HB2	3:A:1420:NAG:O7	2.01	0.60
1:A:200:ARG:HB2	1:A:206:ASP:HB3	1.83	0.60
1:B:321:PHE:CE1	1:B:331:ASN:HB2	2.37	0.60
1:B:471:GLY:HA2	1:B:474:SER:HB3	1.83	0.59
1:B:82:ILE:HD12	1:B:213:ALA:HB1	1.84	0.59
1:A:70:ASN:HB3	1:A:72:VAL:HG12	1.85	0.59
1:A:82:ILE:HD11	1:A:120:LEU:HG	1.84	0.58
1:A:110:GLU:HG2	1:A:112:PRO:HD3	1.86	0.58
1:B:295:GLU:HG2	1:B:296:GLU:H	1.68	0.58
1:B:245:LEU:HG	1:B:256:ASN:HB2	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:352:PHE:CZ	1:A:387:PRO:HD3	2.38	0.57
1:B:532:ILE:HG21	1:B:550:ARG:HG2	1.86	0.57
1:B:124:VAL:H	1:B:152:MET:HG2	1.70	0.57
1:B:496:PRO:HB2	1:B:510:GLU:HG3	1.85	0.57
1:B:62:ALA:O	1:B:84:ARG:HB2	2.04	0.56
2:D:45:ARG:HH22	2:D:51:GLU:HB2	1.69	0.56
1:A:552:PRO:HB2	1:A:567:CYS:H	1.70	0.56
1:B:84:ARG:HD3	1:B:120:LEU:HD12	1.86	0.56
1:B:123:ALA:HB1	1:B:152:MET:HG2	1.87	0.56
1:B:552:PRO:HB2	1:B:567:CYS:H	1.69	0.56
1:B:507:ARG:NH2	1:B:516:LYS:HG3	2.20	0.56
1:B:186:LEU:HD22	1:B:190:ILE:HD11	1.88	0.56
1:A:138:ILE:HG12	1:A:176:TRP:CE2	2.40	0.56
1:B:326:SER:HB2	1:B:348:LEU:HD22	1.87	0.56
1:A:447:TYR:OH	1:A:494:PRO:HG3	2.06	0.55
1:A:6:VAL:HG12	1:A:36:VAL:HB	1.88	0.55
1:B:135:VAL:HA	1:B:138:ILE:HD13	1.88	0.55
1:A:47:GLN:HA	1:A:71:THR:OG1	2.06	0.55
1:A:507:ARG:HH12	1:A:516:LYS:HE3	1.70	0.55
1:A:82:ILE:HG21	1:A:226:VAL:HG11	1.88	0.54
1:A:446:CYS:SG	1:A:470:ARG:HG2	2.48	0.54
1:A:549:GLY:HA3	1:A:554:ASN:OD1	2.08	0.54
1:A:386:TRP:CG	1:A:387:PRO:HD2	2.43	0.53
1:B:117:GLN:HB2	1:B:214:ALA:HB1	1.91	0.53
1:B:563:ASP:HA	1:B:593:CYS:HB2	1.91	0.53
1:B:294:MET:HG2	1:B:303:LYS:HD2	1.90	0.53
1:A:46:VAL:HG12	1:A:72:VAL:HB	1.91	0.53
1:B:134:ASN:OD1	1:B:177:GLY:HA2	2.09	0.53
1:A:515:CYS:SG	1:A:526:VAL:HG22	2.49	0.53
1:B:419:LEU:HD13	1:B:421:ILE:HD11	1.91	0.53
1:B:102:ASP:HB2	1:B:106:THR:O	2.08	0.52
1:A:507:ARG:NH2	1:A:516:LYS:HG3	2.24	0.52
1:B:611:GLY:O	1:B:613:PRO:HD3	2.08	0.52
1:B:447:TYR:HH	1:B:494:PRO:HG3	1.75	0.52
1:A:115:ASN:O	1:A:117:GLN:HG3	2.09	0.52
1:B:6:VAL:HG12	1:B:36:VAL:HB	1.89	0.52
1:B:378:THR:O	1:B:403:ARG:HB2	2.10	0.52
1:A:507:ARG:HD3	1:A:531:CYS:HB2	1.91	0.52
1:A:16:GLN:HB2	1:A:45:TYR:CE1	2.45	0.52
1:A:303:LYS:O	1:A:304:LYS:HD3	2.10	0.52
1:B:485:LEU:HD13	1:B:512:VAL:HA	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:335:PHE:HA	1:A:338:CYS:SG	2.51	0.51
1:A:235:THR:OG1	1:A:237:LYS:HE3	2.11	0.51
1:A:388:GLU:CD	1:A:388:GLU:H	2.13	0.51
1:B:92:SER:OG	3:B:1151:NAG:H4	2.10	0.51
1:B:459:THR:HG22	1:B:460:SER:H	1.76	0.51
1:A:408:GLN:C	1:A:410:GLY:H	2.14	0.51
1:A:36:VAL:HG22	1:A:60:GLU:HG3	1.92	0.51
1:A:505:VAL:HG12	1:A:529:SER:HA	1.92	0.51
1:B:407:LYS:HD3	1:B:435:GLY:HA2	1.92	0.51
1:A:262:SER:H	1:A:282:SER:HA	1.76	0.51
1:B:521:GLU:CB	1:B:522:PRO:HD3	2.36	0.50
1:B:545:ILE:HG13	1:B:556:ILE:HD11	1.94	0.50
1:B:262:SER:HB2	1:B:282:SER:HB3	1.93	0.50
1:A:186:LEU:H	1:A:186:LEU:HD12	1.77	0.50
2:D:48:LYS:O	2:D:49:TRP:CD2	2.65	0.50
2:D:22:TYR:HB2	2:D:29:TYR:CE2	2.47	0.50
1:B:421:ILE:HG22	1:B:423:SER:H	1.76	0.50
1:A:33:ASN:OD1	3:A:1032:NAG:H61	2.12	0.50
1:B:56:LYS:HG2	1:B:76:PRO:HB2	1.94	0.49
1:B:515:CYS:SG	1:B:526:VAL:HG22	2.52	0.49
1:A:505:VAL:HG23	1:A:512:VAL:HG23	1.94	0.49
1:A:327:ILE:HD11	1:A:332:ILE:HG13	1.95	0.49
1:A:245:LEU:HG	1:A:256:ASN:HB2	1.94	0.49
1:B:119:ILE:HG13	1:B:143:ILE:HG22	1.94	0.49
1:A:315:GLY:O	1:A:318:ILE:HG22	2.12	0.49
1:A:88:TYR:OH	1:A:121:HIS:HB3	2.13	0.49
2:D:45:ARG:CG	2:D:45:ARG:NH1	2.75	0.49
1:A:186:LEU:HB2	1:A:190:ILE:HD11	1.95	0.49
1:B:417:VAL:HA	1:B:440:SER:O	2.13	0.48
1:B:507:ARG:HD3	1:B:531:CYS:HB2	1.95	0.48
1:A:597:HIS:HB2	1:A:608:GLY:HA2	1.94	0.48
1:A:409:HIS:CE1	2:C:38:ILE:HD11	2.48	0.48
1:A:114:ARG:HD3	1:A:182:ASN:OD1	2.13	0.48
1:A:142:ASP:CG	1:A:188:LYS:HB3	2.33	0.48
1:A:49:ASN:O	1:A:50:TYR:O	2.31	0.48
1:A:459:THR:O	1:A:462:GLN:HG3	2.14	0.48
1:A:119:ILE:HG13	1:A:143:ILE:HG22	1.95	0.48
1:B:525:PHE:CE2	1:B:532:ILE:HB	2.49	0.47
1:B:101:TYR:HE2	1:B:128:ASN:HB3	1.79	0.47
1:B:399:LEU:HD22	1:B:429:LEU:HD13	1.95	0.47
1:B:419:LEU:HB3	1:B:421:ILE:HG13	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:262:SER:H	1:B:282:SER:HA	1.79	0.47
1:B:10:THR:O	1:B:40:ASN:HB2	2.14	0.47
1:B:295:GLU:HG2	1:B:296:GLU:N	2.28	0.47
1:B:383:ILE:HG22	1:B:419:LEU:HD11	1.96	0.47
1:A:303:LYS:NZ	1:A:303:LYS:HB3	2.30	0.47
1:A:125:ARG:HD2	1:A:153:SER:O	2.13	0.47
1:B:459:THR:HG22	1:B:460:SER:N	2.29	0.47
1:B:114:ARG:HA	1:B:176:TRP:CD1	2.49	0.47
1:B:15:THR:HG23	2:D:31:CYS:O	2.14	0.47
1:B:47:GLN:HA	1:B:71:THR:OG1	2.15	0.47
1:A:295:GLU:CG	1:A:300:ARG:HH11	2.28	0.47
1:B:296:GLU:C	1:B:298:GLY:H	2.18	0.47
1:B:269:LYS:N	1:B:269:LYS:HD3	2.29	0.47
1:A:276:VAL:HG11	1:A:302:CYS:SG	2.55	0.47
1:B:82:ILE:HD11	1:B:120:LEU:HG	1.97	0.47
1:A:32:ASN:O	1:A:33:ASN:HB2	2.13	0.47
1:A:397:GLU:HG3	1:A:427:ARG:NH1	2.30	0.47
1:B:89:TYR:CE2	1:B:90:GLU:HG2	2.51	0.46
1:B:132:LEU:HD11	1:B:135:VAL:HG21	1.98	0.46
1:A:386:TRP:CD2	1:A:387:PRO:HD2	2.50	0.46
1:A:470:ARG:HG2	1:A:475:CYS:SG	2.55	0.46
1:A:288:GLY:C	1:A:290:ASP:H	2.18	0.46
1:B:330:THR:O	1:B:333:LYS:HG3	2.16	0.46
1:A:190:ILE:O	1:A:190:ILE:HG22	2.15	0.46
1:B:473:ASN:O	1:B:476:LYS:HG2	2.15	0.46
1:A:69:LEU:HD11	2:C:23:ILE:HD13	1.97	0.46
4:D:1:2PE:H172	4:D:1:2PE:H142	1.62	0.46
1:B:110:GLU:HG2	1:B:112:PRO:HG3	1.97	0.46
1:B:403:ARG:O	1:B:433:SER:HB2	2.16	0.46
1:B:246:TYR:O	1:B:248:PRO:HD3	2.15	0.46
1:B:75:ILE:HA	1:B:76:PRO:HD3	1.77	0.46
1:A:397:GLU:HG3	1:A:427:ARG:HH11	1.80	0.46
1:A:350:VAL:HG22	1:A:355:ASP:HB2	1.98	0.46
1:B:393:LEU:HG	1:B:421:ILE:HD13	1.98	0.45
1:A:408:GLN:C	1:A:410:GLY:N	2.69	0.45
1:A:390:ARG:HG3	1:A:394:HIS:CE1	2.50	0.45
1:B:532:ILE:N	1:B:532:ILE:HD12	2.32	0.45
1:B:487:SER:HB3	1:B:501:SER:OG	2.17	0.45
1:B:447:TYR:CZ	1:B:494:PRO:HG3	2.51	0.45
1:B:27:LEU:HD21	1:B:43:ILE:HG23	1.97	0.45
1:A:102:ASP:HB2	1:A:106:THR:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:352:PHE:CZ	1:B:387:PRO:HD3	2.51	0.45
1:B:296:GLU:C	1:B:298:GLY:N	2.70	0.45
1:B:416:VAL:HB	1:B:439:ILE:HG23	1.98	0.45
1:B:442:ASN:O	1:B:469:ASN:HA	2.17	0.45
1:B:296:GLU:CD	1:B:297:ASP:H	2.21	0.44
1:B:327:ILE:O	1:B:327:ILE:HG23	2.17	0.44
1:A:532:ILE:HD12	1:A:532:ILE:N	2.32	0.44
1:B:186:LEU:HD23	1:B:189:ILE:HD11	2.00	0.44
1:A:248:PRO:HG3	1:B:230:PHE:CZ	2.52	0.44
1:B:324:SER:HB3	3:B:1328:NAG:H4	1.99	0.44
1:B:295:GLU:HB2	1:B:300:ARG:HH11	1.82	0.44
1:A:36:VAL:HG22	1:A:60:GLU:CG	2.47	0.44
1:A:253:MET:HE2	1:A:253:MET:HB2	1.67	0.44
1:A:246:TYR:O	1:A:248:PRO:HD3	2.18	0.44
1:B:388:GLU:H	1:B:388:GLU:CD	2.21	0.44
1:A:330:THR:O	1:A:333:LYS:HG3	2.17	0.44
1:A:295:GLU:HG3	1:A:300:ARG:NH1	2.33	0.44
1:B:115:ASN:O	1:B:117:GLN:HG3	2.18	0.43
1:A:478:THR:O	1:A:478:THR:HG22	2.18	0.43
1:A:611:GLY:O	1:A:613:PRO:HD3	2.18	0.43
1:A:262:SER:HB2	1:A:282:SER:CB	2.48	0.43
1:B:29:ARG:HB3	2:D:49:TRP:CZ2	2.53	0.43
1:B:142:ASP:CG	1:B:188:LYS:HB3	2.38	0.43
1:A:485:LEU:HD13	1:A:512:VAL:HA	2.00	0.43
1:A:186:LEU:HB2	1:A:190:ILE:CD1	2.48	0.43
1:B:516:LYS:CD	1:B:522:PRO:HD2	2.48	0.43
1:A:67:ILE:HG22	1:A:100:ASN:HD21	1.84	0.43
1:B:200:ARG:HH12	1:B:219:PRO:HD3	1.84	0.43
1:A:75:ILE:HA	1:A:76:PRO:HD3	1.81	0.42
1:B:585:LYS:HG2	1:B:595:LEU:HA	2.01	0.42
1:A:12:ASN:HB3	1:A:15:THR:HB	2.01	0.42
1:B:360:THR:HA	1:B:361:PRO:HD3	1.84	0.42
1:A:296:GLU:O	1:A:297:ASP:HB2	2.20	0.42
1:B:386:TRP:CG	1:B:387:PRO:HD2	2.55	0.42
1:B:424:LEU:HD13	1:B:492:TRP:HZ3	1.84	0.42
1:A:72:VAL:HG22	1:A:73:GLU:N	2.34	0.42
1:B:117:GLN:O	1:B:143:ILE:HA	2.19	0.42
1:A:262:SER:HB2	1:A:282:SER:HB3	2.01	0.42
1:A:101:TYR:HB3	1:A:130:PRO:HD2	2.01	0.42
1:A:360:THR:HA	1:A:361:PRO:HD3	1.89	0.42
1:B:344:ASP:OD1	1:B:379:GLY:HA3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:1151:NAG:H3	3:B:1151:NAG:O7	2.19	0.42
1:A:295:GLU:HG3	1:A:300:ARG:HH11	1.83	0.42
1:B:492:TRP:N	1:B:498:ASP:O	2.52	0.42
1:A:561:TYR:HA	1:A:591:HIS:HB3	2.01	0.42
1:A:487:SER:OG	1:A:488:PRO:HD2	2.20	0.42
1:B:98:LEU:O	1:B:99:SER:C	2.58	0.42
1:B:194:GLN:NE2	1:B:204:PRO:HB3	2.31	0.41
1:A:287:CYS:SG	1:A:293:GLU:HG2	2.60	0.41
1:A:35:GLU:HA	1:A:57:THR:O	2.20	0.41
1:A:525:PHE:CE2	1:A:532:ILE:HB	2.55	0.41
1:B:188:LYS:HB2	1:B:198:ARG:NH1	2.35	0.41
1:A:126:PHE:HB2	1:A:154:MET:HB2	2.01	0.41
1:A:126:PHE:H	1:A:154:MET:HB3	1.84	0.41
1:B:288:GLY:C	1:B:290:ASP:H	2.22	0.41
1:A:521:GLU:CB	1:A:522:PRO:HD3	2.35	0.41
1:B:467:ILE:HD11	2:D:51:GLU:H	1.86	0.41
1:A:507:ARG:NH1	1:A:516:LYS:HE3	2.35	0.41
1:A:134:ASN:OD1	1:A:177:GLY:HA2	2.21	0.41
1:B:101:TYR:HB3	1:B:130:PRO:HD2	2.02	0.41
1:B:28:GLN:O	1:B:32:ASN:HB2	2.20	0.41
1:A:269:LYS:HD3	1:A:269:LYS:N	2.35	0.41
1:B:111:LEU:HG	1:B:113:MET:HG3	2.03	0.41
1:B:82:ILE:HG21	1:B:226:VAL:HG11	2.02	0.41
1:A:177:GLY:HA3	1:A:182:ASN:HD22	1.86	0.41
1:A:582:LEU:HD12	1:A:582:LEU:N	2.36	0.41
1:B:218:GLY:N	1:B:223:ASP:HB3	2.36	0.41
1:B:89:TYR:CD2	1:B:90:GLU:HG2	2.56	0.41
1:B:138:ILE:HG22	1:B:140:TRP:CD1	2.56	0.40
1:A:495:GLU:HA	1:A:496:PRO:HD3	1.94	0.40
2:D:19:VAL:CG2	2:D:32:ASN:HB3	2.51	0.40
1:A:83:ILE:O	1:A:119:ILE:HA	2.22	0.40
1:A:380:PHE:C	1:A:380:PHE:CD1	2.94	0.40
1:A:144:VAL:HG12	1:A:145:SER:N	2.36	0.40
1:B:262:SER:HB2	1:B:282:SER:CB	2.51	0.40
1:A:68:ALA:HA	1:A:98:LEU:O	2.22	0.40
1:B:350:VAL:HG22	1:B:355:ASP:HB2	2.03	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	613/614 (100%)	531 (87%)	78 (13%)	4 (1%)	26	66
1	B	613/614 (100%)	531 (87%)	77 (13%)	5 (1%)	24	62
2	C	45/47 (96%)	40 (89%)	4 (9%)	1 (2%)	8	41
2	D	45/47 (96%)	40 (89%)	4 (9%)	1 (2%)	8	41
All	All	1316/1322 (100%)	1142 (87%)	163 (12%)	11 (1%)	24	62

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	50	TYR
1	A	336	LYS
1	B	99	SER
1	B	295	GLU
2	D	46	ASP
1	A	443	LYS
1	B	336	LYS
1	B	296	GLU
2	C	50	TRP
1	A	540	PRO
1	B	494	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	537/536 (100%)	537 (100%)	0	100 100
1	B	537/536 (100%)	536 (100%)	1 (0%)	95 98
2	C	41/41 (100%)	41 (100%)	0	100 100
2	D	41/41 (100%)	40 (98%)	1 (2%)	57 83
All	All	1156/1154 (100%)	1154 (100%)	2 (0%)	95 98

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	290	ASP
2	D	50	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	157	GLN
1	A	409	HIS
1	B	33	ASN
1	B	194	GLN
1	B	280	HIS
1	B	408	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

17 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	$\#\|Z\| > 2$
3	NAG	A	1032	1	14,14,15	0.46	0	15,19,21	1.16	1 (6%)
3	NAG	A	1049	1	14,14,15	0.54	0	15,19,21	0.61	0
3	NAG	A	1151	1	14,14,15	0.45	0	15,19,21	0.94	1 (6%)
3	NAG	A	1172	1	14,14,15	0.49	0	15,19,21	0.81	1 (6%)
3	NAG	A	1328	1	14,14,15	0.47	0	15,19,21	0.84	0
3	NAG	A	1337	1	14,14,15	0.50	0	15,19,21	0.74	0
3	NAG	A	1420	1	14,14,15	0.50	0	15,19,21	0.61	0
3	NAG	A	1504	1	14,14,15	0.48	0	15,19,21	0.75	1 (6%)
3	NAG	B	1032	1	14,14,15	0.46	0	15,19,21	0.97	1 (6%)
3	NAG	B	1151	1	14,14,15	0.44	0	15,19,21	0.81	1 (6%)
3	NAG	B	1328	1	14,14,15	0.47	0	15,19,21	0.90	0
3	NAG	B	1504	1	14,14,15	0.49	0	15,19,21	0.73	1 (6%)
4	2PE	B	615	-	27,27,27	0.55	0	26,26,26	0.38	0
4	2PE	B	616	-	27,27,27	0.53	0	26,26,26	0.32	0
4	2PE	B	617	-	27,27,27	0.55	0	26,26,26	0.29	0
4	2PE	D	1	-	27,27,27	0.51	0	26,26,26	0.30	0
4	2PE	D	52	-	27,27,27	0.54	0	26,26,26	0.34	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	A	1032	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1049	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1151	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1172	1	1/1/5/7	0/6/23/26	0/1/1/1
3	NAG	A	1328	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1337	1	1/1/5/7	0/6/23/26	0/1/1/1
3	NAG	A	1420	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1504	1	-	0/6/23/26	0/1/1/1
3	NAG	B	1032	1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	B	1151	1	-	0/6/23/26	0/1/1/1
3	NAG	B	1328	1	-	0/6/23/26	0/1/1/1
3	NAG	B	1504	1	1/1/5/7	0/6/23/26	0/1/1/1
4	2PE	B	615	-	-	0/25/25/25	0/0/0/0
4	2PE	B	616	-	-	0/25/25/25	0/0/0/0
4	2PE	B	617	-	-	0/25/25/25	0/0/0/0
4	2PE	D	1	-	-	0/25/25/25	0/0/0/0
4	2PE	D	52	-	-	0/25/25/25	0/0/0/0

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1504	NAG	C1-O5-C5	2.02	114.81	112.25
3	B	1504	NAG	C1-O5-C5	2.05	114.85	112.25
3	B	1151	NAG	C1-O5-C5	2.20	115.05	112.25
3	A	1172	NAG	C1-O5-C5	2.31	115.18	112.25
3	A	1151	NAG	C1-O5-C5	2.45	115.35	112.25
3	B	1032	NAG	C1-O5-C5	2.82	115.83	112.25
3	A	1032	NAG	C1-O5-C5	3.84	117.13	112.25

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	1172	NAG	C1
3	A	1337	NAG	C1
3	B	1504	NAG	C1

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1032	NAG	1	0
3	A	1420	NAG	1	0
3	B	1151	NAG	2	0
3	B	1328	NAG	1	0
4	B	616	2PE	1	0
4	B	617	2PE	1	0
4	D	1	2PE	1	0

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^{th} 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	614/614 (100%)	0.52	55 (8%) 12 9	70, 110, 241, 303	0
1	B	614/614 (100%)	0.37	55 (8%) 12 9	65, 117, 222, 268	0
2	C	47/47 (100%)	0.13	0 100 100	81, 98, 131, 163	0
2	D	47/47 (100%)	0.08	2 (4%) 39 32	81, 111, 154, 184	0
All	All	1322/1322 (100%)	0.42	112 (8%) 13 10	65, 113, 228, 303	0

All (112) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	573	ALA	11.5
1	A	605	THR	10.8
1	A	587	ALA	9.7
1	A	589	ALA	8.6
1	A	588	ASP	8.4
1	B	578	GLU	8.4
1	B	572	PRO	7.6
1	B	574	GLY	7.5
1	B	601	THR	7.4
1	A	602	TYR	7.0
1	A	570	THR	6.9
1	A	601	THR	6.8
1	A	574	GLY	6.5
1	B	591	HIS	5.5
1	B	573	ALA	5.5
1	A	591	HIS	5.3
1	B	583	VAL	5.3
1	B	579	ASN	5.3
1	B	575	VAL	5.2
1	A	590	GLY	5.0
1	A	545	ILE	4.9

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Mol	Chain	Res	Type	RSRZ
1	A	526	VAL	4.7
1	A	613	PRO	4.6
1	B	597	HIS	4.5
1	A	571	CYS	4.5
1	A	612	CYS	4.4
1	A	556	ILE	4.4
1	A	575	VAL	4.4
1	B	543	MET	4.2
1	B	565	PRO	4.0
1	B	526	VAL	4.0
1	A	525	PHE	4.0
1	B	582	LEU	4.0
1	B	485	LEU	3.9
1	A	543	MET	3.9
1	A	533	GLN	3.9
1	B	566	HIS	3.9
1	B	599	ASN	3.9
1	A	578	GLU	3.9
1	B	545	ILE	3.7
1	B	598	PRO	3.7
1	A	561	TYR	3.7
1	A	603	GLY	3.6
1	A	562	ILE	3.6
1	B	531	CYS	3.6
1	A	572	PRO	3.6
1	B	593	CYS	3.5
1	A	581	THR	3.5
1	A	214	ALA	3.4
1	B	592	VAL	3.4
1	B	523	ARG	3.4
1	B	590	GLY	3.3
1	A	610	GLU	3.3
1	B	576	MET	3.3
1	A	306	GLU	3.2
1	A	599	ASN	3.2
1	B	158	ASN	3.2
1	B	521	GLU	3.2
1	A	308	PRO	3.2
1	A	614	THR	3.2
1	A	611	GLY	3.1
1	B	507	ARG	3.1
1	B	280	HIS	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	542	ALA	3.0
1	B	194	GLN	3.0
1	A	550	ARG	2.9
1	B	569	LYS	2.9
1	B	581	THR	2.8
1	A	579	ASN	2.8
1	A	597	HIS	2.8
1	B	589	ALA	2.7
1	A	549	GLY	2.7
1	B	525	PHE	2.6
1	A	577	GLY	2.6
1	B	530	GLU	2.6
1	B	548	THR	2.5
1	B	449	ASN	2.5
1	A	202	LYS	2.5
1	A	532	ILE	2.5
1	B	570	THR	2.5
1	B	584	TRP	2.4
1	B	605	THR	2.4
1	B	560	HIS	2.4
1	B	602	TYR	2.4
1	B	202	LYS	2.4
1	A	557	GLN	2.4
1	B	473	ASN	2.3
1	B	515	CYS	2.3
2	D	10	HIS	2.2
1	A	176	TRP	2.2
1	A	201	GLY	2.2
1	A	609	LEU	2.2
1	A	1	LEU	2.2
1	A	205	SER	2.2
1	A	311	LYS	2.2
1	A	548	THR	2.2
1	A	531	CYS	2.1
1	A	604	CYS	2.1
1	B	386	TRP	2.1
1	B	524	GLU	2.1
1	B	561	TYR	2.1
1	B	489	GLU	2.1
1	A	608	GLY	2.1
1	B	559	ALA	2.1
1	B	529	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	556	ILE	2.1
2	D	8	LEU	2.1
1	B	472	GLU	2.1
1	B	186	LEU	2.0
1	B	518	LEU	2.0
1	A	534	CYS	2.0
1	A	200	ARG	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^{th} 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
3	NAG	B	1032	14/15	0.81	0.25	0.93	115,127,138,147	0
3	NAG	A	1151	14/15	0.77	0.28	0.77	101,109,116,119	0
3	NAG	B	1328	14/15	0.94	0.26	0.51	69,81,95,98	0
3	NAG	A	1328	14/15	0.91	0.30	0.36	70,79,88,91	0
3	NAG	A	1172	14/15	0.81	0.17	-1.10	123,135,143,144	0
3	NAG	A	1420	14/15	0.86	0.31	-	144,148,176,178	0
3	NAG	A	1337	14/15	0.84	0.40	-	147,155,158,158	0
4	2PE	B	615	28/28	0.72	0.17	-	88,105,147,157	0
3	NAG	A	1049	14/15	0.75	0.40	-	130,153,165,166	0
4	2PE	D	1	28/28	0.79	0.19	-	116,139,157,157	0
4	2PE	B	617	28/28	0.70	0.21	-	79,97,115,119	0
4	2PE	D	52	28/28	0.74	0.16	-	110,124,137,143	0
4	2PE	B	616	28/28	0.87	0.15	-	84,105,115,118	0
3	NAG	A	1504	14/15	0.87	0.40	-	152,159,166,168	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	NAG	B	1504	14/15	0.83	0.36	-	170,178,191,191	0
3	NAG	A	1032	14/15	0.85	0.22	-	108,120,129,132	0
3	NAG	B	1151	14/15	0.86	0.16	-	142,149,164,165	0

6.5 Other polymers (i)

There are no such residues in this entry.