



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 03:50 PM UTC

PDB ID : 4IGL / pdb_00004igl
Title : Structure of the RHS-repeat containing BC component of the secreted ABC toxin complex from *Yersinia entomophaga*
Authors : Busby, J.N.; Panjikar, S.; Landsberg, M.J.; Hurst, M.R.H.; Lott, J.S.
Deposited on : 2012-12-17
Resolution : 2.49 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

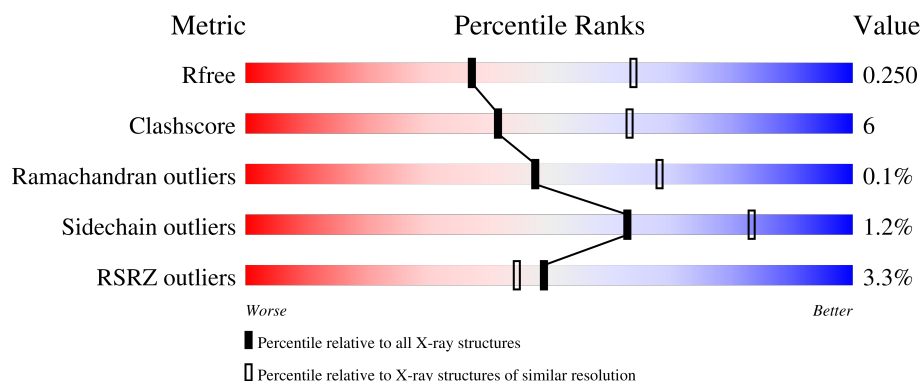
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.49 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}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	1488	 3% 82% 15% ..
1	C	1488	 2% 82% 15% .
2	B	690	 4% 82% 14% .
2	D	690	 4% 79% 17% ..

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 35548 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 YenB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1457	Total	C	N	O	S	0	3	0
			11431	7242	1963	2189	37			
1	C	1449	Total	C	N	O	S	0	4	0
			11370	7196	1948	2189	37			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	expression tag	UNP B6A880
C	0	GLY	-	expression tag	UNP B6A880

- Molecule 2 is a protein called YenC2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	666	Total	C	N	O	S	0	0	0
			5100	3181	886	1022	11			
2	D	668	Total	C	N	O	S	0	1	0
			5126	3201	891	1022	12			

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 6 3 3	0	0
3	A	1	Total C O 6 3 3	0	0
3	C	1	Total C O 6 3 3	0	0
3	C	1	Total C O 6 3 3	0	0
3	C	1	Total C O 6 3 3	0	0
3	C	1	Total C O 6 3 3	0	0
3	C	1	Total C O 6 3 3	0	0
3	D	1	Total C O 6 3 3	0	0

- Molecule 4 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	3	Total K 3 3	0	0
4	C	3	Total K 3 3	0	0

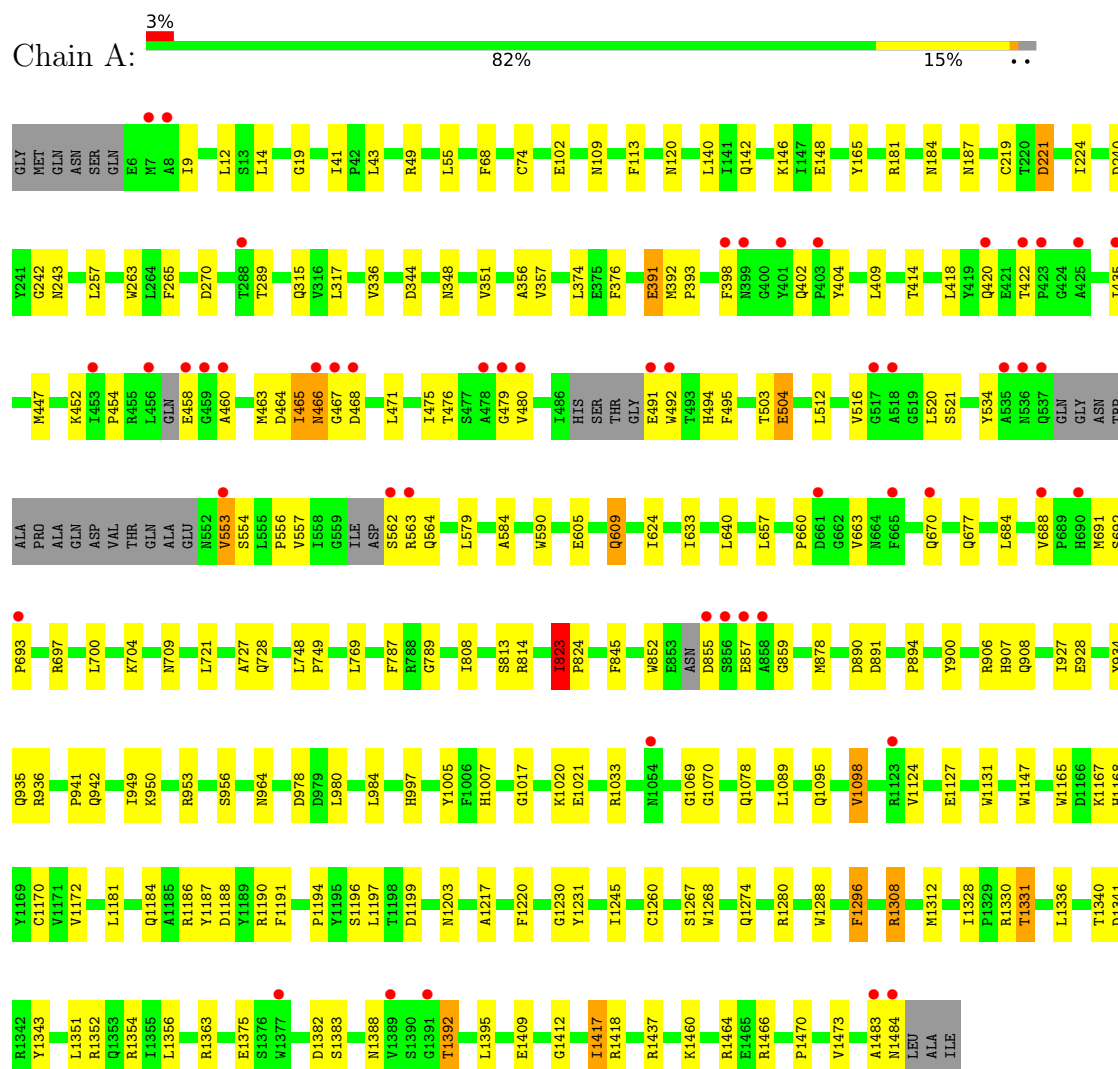
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	880	Total 880	O 880	0	0
5	B	332	Total 332	O 332	0	0
5	C	906	Total 906	O 906	0	0
5	D	349	Total 349	O 349	0	0

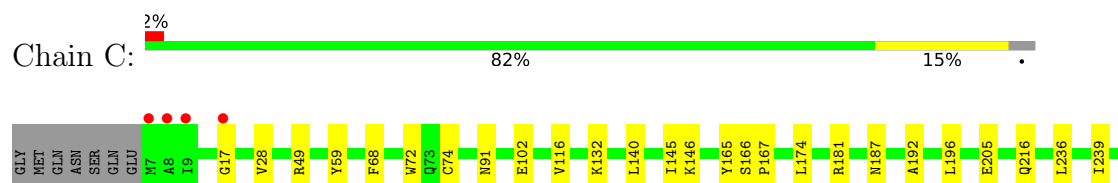
3 Residue-property plots [i](#)

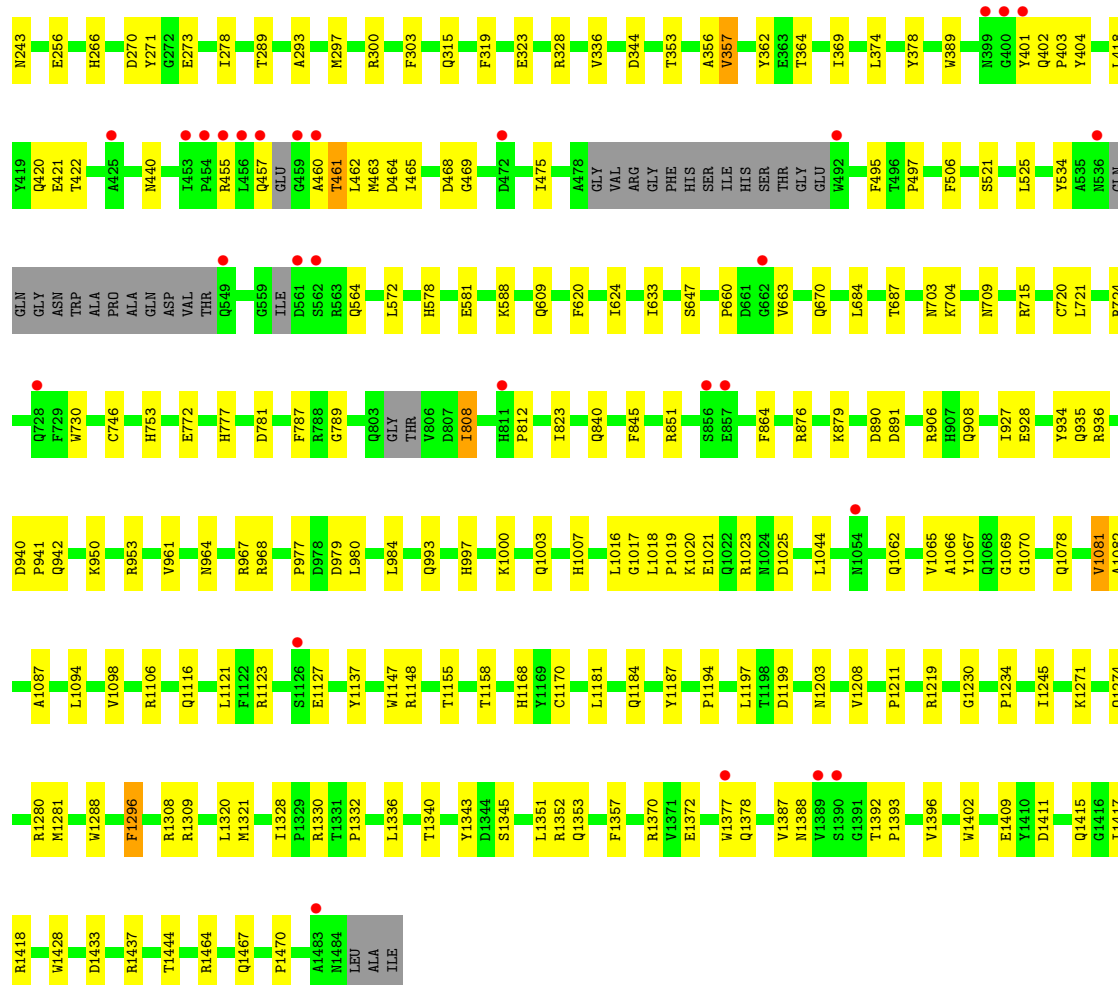
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: YenB

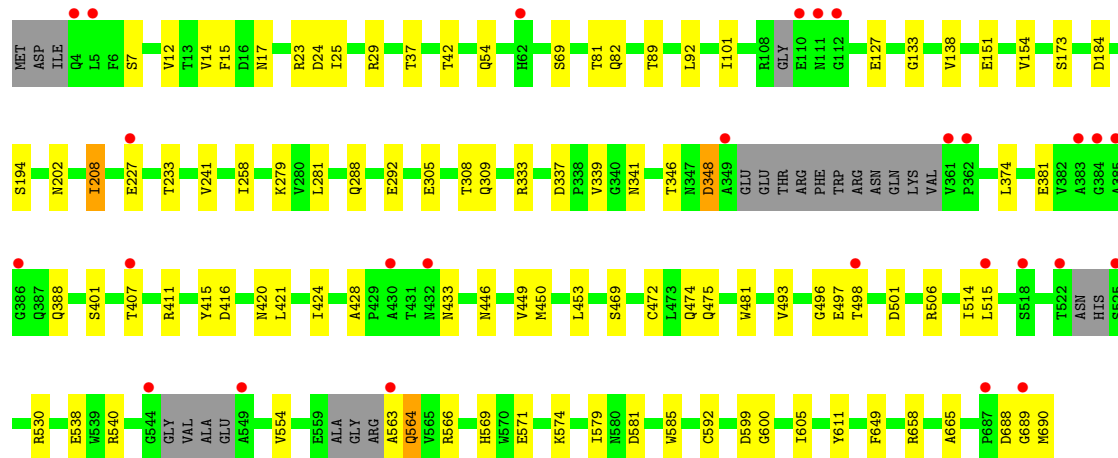
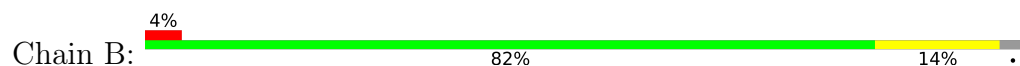


• Molecule 1: YenB

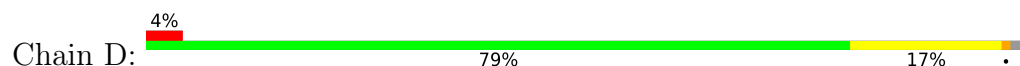


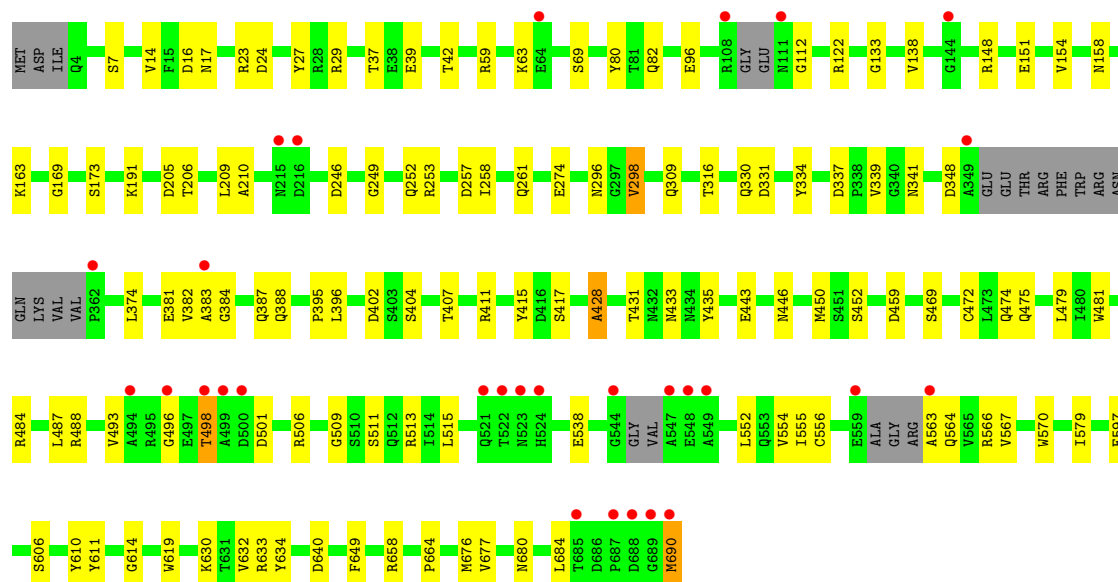


• Molecule 2: YenC2



• Molecule 2: YenC2





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	133.72Å 147.60Å 274.35Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.55 – 2.49 49.55 – 2.49	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.55-2.49) 95.4 (49.55-2.49)	Depositor EDS
R_{merge}	0.30	Depositor
R_{sym}	0.30	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.24 (at 2.27Å)	Xtriage
Refinement program	PHENIX 1.8.1_1168	Depositor
R, R_{free}	0.200 , 0.251 0.202 , 0.250	Depositor DCC
R_{free} test set	12329 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å ²)	29.2	Xtriage
Anisotropy	0.093	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 40.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	35548	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.99% 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: K, GOL

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	0.35	0/11744	0.77	11/16018 (0.1%)
1	C	0.35	0/11683	0.78	11/15938 (0.1%)
2	B	0.34	0/5196	0.74	1/7081 (0.0%)
2	D	0.35	0/5226	0.74	2/7119 (0.0%)
All	All	0.35	0/33849	0.76	25/46156 (0.1%)

There are no bond length outliers.

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	808	ILE	CA-C-N	7.73	129.51	119.84
1	C	808	ILE	C-N-CA	7.73	129.51	119.84
1	A	466	ASN	N-CA-C	7.47	120.08	111.11
1	C	469	GLY	N-CA-C	-6.62	106.18	115.32
1	C	1098	VAL	N-CA-C	6.56	117.05	110.23
2	B	401	SER	N-CA-C	-6.02	106.47	113.88
1	A	465	ILE	N-CA-C	5.92	116.65	111.56
1	A	1296	PHE	N-CA-C	-5.89	104.86	111.28
1	A	1098	VAL	N-CA-C	5.84	116.31	110.23
1	A	823	ILE	CA-C-N	5.84	125.53	119.05
1	A	823	ILE	C-N-CA	5.84	125.53	119.05
2	D	428	ALA	CA-C-N	5.61	125.08	119.24
2	D	428	ALA	C-N-CA	5.61	125.08	119.24
1	C	808	ILE	N-CA-C	5.52	113.51	107.60
1	C	401	TYR	N-CA-C	-5.50	106.57	113.72
1	A	1328	ILE	N-CA-C	5.47	113.28	107.76
1	A	1392	THR	CA-C-N	5.39	125.66	119.83
1	A	1392	THR	C-N-CA	5.39	125.66	119.83
1	C	187	ASN	CA-C-N	5.22	124.89	119.56
1	C	187	ASN	C-N-CA	5.22	124.89	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	1328	ILE	N-CA-C	5.17	112.98	107.76
1	C	461	THR	N-CA-C	5.15	117.24	109.41
1	C	1296	PHE	N-CA-C	-5.08	105.74	111.28
1	A	422	THR	CA-C-N	5.07	139.18	127.00
1	A	422	THR	C-N-CA	5.07	139.18	127.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	11431	0	10793	135	0
1	C	11370	0	10711	153	0
2	B	5100	0	4844	54	0
2	D	5126	0	4894	81	0
3	A	12	0	16	1	0
3	C	30	0	40	2	0
3	D	6	0	8	1	0
4	A	3	0	0	0	0
4	C	3	0	0	0	0
5	A	880	0	0	15	0
5	B	332	0	0	7	0
5	C	906	0	0	33	0
5	D	349	0	0	13	0
All	All	35548	0	31306	411	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 6.

All (411) 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:49:ARG:NH2	1:A:243:ASN:O	2.15	0.80
2:D:14:VAL:HB	2:D:23:ARG:HB2	1.65	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:14:VAL:HB	2:B:23:ARG:HB2	1.62	0.79
2:D:472:CYS:SG	5:D:995:HOH:O	2.42	0.76
1:C:1271:LYS:NZ	5:C:1946:HOH:O	2.19	0.74
1:C:49:ARG:NH2	1:C:243:ASN:O	2.20	0.74
2:B:7:SER:O	2:B:29:ARG:NH2	2.18	0.73
1:A:1267:SER:HB2	1:A:1331:THR:HG23	1.72	0.72
2:D:7:SER:O	2:D:29:ARG:NH2	2.23	0.71
2:B:472:CYS:SG	5:B:925:HOH:O	2.48	0.69
1:C:1377:TRP:NE1	5:C:2247:HOH:O	2.26	0.69
2:B:446:ASN:O	2:B:658:ARG:NH1	2.26	0.68
1:A:557:VAL:O	1:A:564:GLN:NE2	2.25	0.68
2:D:452:SER:O	2:D:475:GLN:NE2	2.27	0.68
2:D:29:ARG:NH1	2:D:37:THR:OG1	2.26	0.67
2:D:122:ARG:NH2	5:D:1100:HOH:O	2.27	0.67
2:D:253:ARG:NH2	5:D:1127:HOH:O	2.27	0.67
1:C:1330:ARG:NH1	5:C:1858:HOH:O	2.28	0.66
1:C:720:CYS:SG	5:C:2457:HOH:O	2.52	0.66
2:D:191:LYS:NZ	5:D:1108:HOH:O	2.28	0.66
1:A:677:GLN:O	1:A:728:GLN:NE2	2.29	0.66
1:A:1020:LYS:HG2	1:A:1021:GLU:HG3	1.79	0.65
1:C:49:ARG:HG2	1:C:1170:CYS:HA	1.76	0.65
1:A:624:ILE:HD11	1:A:633:ILE:HD11	1.79	0.65
2:B:288:GLN:OE1	2:B:309:GLN:NE2	2.28	0.65
1:C:1411:ASP:HB3	1:C:1417:ILE:HD11	1.79	0.65
1:A:492:TRP:O	5:A:2333:HOH:O	2.14	0.65
1:C:624:ILE:HD11	1:C:633:ILE:HD11	1.77	0.64
1:C:720:CYS:SG	5:C:2329:HOH:O	2.54	0.64
1:C:942:GLN:NE2	2:D:17:ASN:HA	2.13	0.64
1:A:49:ARG:HG2	1:A:1170:CYS:HA	1.80	0.64
1:C:205:GLU:OE2	1:C:1148[A]:ARG:NH2	2.30	0.64
2:D:39:GLU:OE2	5:D:1098:HOH:O	2.15	0.64
1:C:440:ASN:OD1	1:C:724:ARG:NH1	2.31	0.64
1:C:1020:LYS:HG2	1:C:1021:GLU:HG3	1.80	0.64
1:A:942:GLN:NE2	2:B:17:ASN:HA	2.13	0.63
1:C:1409:GLU:HB3	1:C:1418:ARG:HB2	1.79	0.63
2:D:402:ASP:OD1	2:D:404:SER:N	2.30	0.63
1:A:1466:ARG:NH1	5:A:1947:HOH:O	2.30	0.63
2:D:484:ARG:NH2	2:D:509:GLY:O	2.31	0.63
2:D:513:ARG:NH1	2:D:640:ASP:OD2	2.29	0.63
1:C:369:ILE:HD13	1:C:1211:PRO:HD2	1.81	0.62
1:C:270:ASP:HB3	1:C:315:GLN:HB2	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:102:GLU:HG2	1:C:140:LEU:H	1.66	0.61
2:D:566:ARG:HH22	2:D:632:VAL:HG21	1.64	0.61
1:C:146:LYS:HB3	1:C:165:TYR:HB2	1.82	0.61
1:A:1069:GLY:N	1:A:1070:GLY:HA3	2.15	0.60
1:C:950:LYS:NZ	5:C:2261:HOH:O	2.32	0.60
1:A:894:PRO:O	5:A:2433:HOH:O	2.16	0.60
1:C:715:ARG:NH2	5:C:2334:HOH:O	2.24	0.60
1:C:181:ARG:NH1	5:C:1691:HOH:O	2.28	0.60
1:A:709:ASN:HA	1:A:721:LEU:HB2	1.83	0.60
1:A:1388:ASN:HD21	1:A:1392:THR:HB	1.66	0.59
2:B:450:MET:HE1	2:B:474:GLN:HG2	1.84	0.59
1:A:146:LYS:HB3	1:A:165:TYR:HB2	1.84	0.59
1:C:588:LYS:NZ	5:C:2163:HOH:O	2.27	0.59
1:C:1069:GLY:N	1:C:1070:GLY:HA3	2.18	0.59
1:C:49:ARG:NH1	1:C:1168:HIS:O	2.35	0.59
1:A:398:PHE:HD2	1:A:402:GLN:HG2	1.65	0.59
2:D:446:ASN:O	2:D:658:ARG:NH1	2.34	0.59
2:D:506:ARG:HB2	2:D:515:LEU:HB3	1.85	0.59
1:C:1309:ARG:NH1	5:C:2360:HOH:O	2.36	0.58
2:D:383:ALA:HB2	2:D:407:THR:OG1	2.02	0.58
2:B:24:ASP:OD1	5:B:1020:HOH:O	2.17	0.58
1:A:878:MET:HE3	1:A:907:HIS:HB2	1.85	0.58
1:C:704:LYS:HG3	1:C:753:HIS:CE1	2.38	0.58
1:C:1137:TYR:OH	5:C:2370:HOH:O	2.16	0.58
1:A:980:LEU:HD13	1:A:984:LEU:HD23	1.84	0.58
2:D:555:ILE:HB	2:D:567:VAL:HB	1.86	0.58
2:B:538:GLU:HB2	2:B:554:VAL:HB	1.86	0.57
1:C:753:HIS:ND1	5:C:1964:HOH:O	2.33	0.57
1:A:270:ASP:HB3	1:A:315:GLN:HB2	1.86	0.57
2:D:205:ASP:O	2:D:506:ARG:NH1	2.37	0.57
1:C:521:SER:N	1:C:534:TYR:O	2.38	0.57
1:C:808:ILE:HD13	1:C:1417:ILE:HG21	1.86	0.57
1:A:1464:ARG:NH1	5:A:1792:HOH:O	2.36	0.56
2:D:24:ASP:HB2	2:D:42:THR:HB	1.85	0.56
1:C:300:ARG:NH2	5:C:1925:HOH:O	2.35	0.56
1:C:980:LEU:HD13	1:C:984:LEU:HD23	1.88	0.56
2:D:493:VAL:HB	2:D:501:ASP:HB2	1.87	0.56
1:A:813:SER:HB3	3:A:1502:GOL:H11	1.88	0.56
1:A:49:ARG:NH1	1:A:1168:HIS:O	2.37	0.56
2:B:337:ASP:OD1	2:B:341:ASN:N	2.35	0.56
1:C:660:PRO:HG2	1:C:663:VAL:HG21	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1078:GLN:HG2	1:A:1147:TRP:CD2	2.40	0.55
1:C:344:ASP:HB2	1:C:356:ALA:HB3	1.86	0.55
2:D:63:LYS:NZ	2:D:443:GLU:OE1	2.37	0.55
2:B:665:ALA:HB2	2:B:690:MET:HG3	1.88	0.55
2:D:138:VAL:HB	2:D:151:GLU:HB2	1.88	0.55
1:C:463:MET:HE2	1:C:465:ILE:HG13	1.88	0.55
1:C:940:ASP:OD2	1:C:967:ARG:NH2	2.33	0.55
1:A:464:ASP:HB2	1:A:471:LEU:HD12	1.89	0.55
1:A:1340:THR:HG22	1:A:1351:LEU:HD22	1.87	0.55
1:A:852:TRP:HE1	1:A:855:ASP:HB2	1.73	0.54
1:A:466:ASN:N	1:A:467:GLY:HA2	2.23	0.54
1:C:1464:ARG:NH1	5:C:1855:HOH:O	2.41	0.54
1:A:1409:GLU:HB3	1:A:1418:ARG:HB2	1.89	0.54
1:C:1467:GLN:NE2	5:C:2431:HOH:O	2.40	0.54
2:B:506:ARG:HB2	2:B:515:LEU:HB3	1.89	0.54
1:C:1062:GLN:HG2	1:C:1087:ALA:HB2	1.89	0.54
1:A:398:PHE:CD2	1:A:402:GLN:HG2	2.42	0.54
1:A:908:GLN:HB2	1:A:927:ILE:HD13	1.90	0.54
1:C:463:MET:SD	1:C:475:ILE:HD11	2.47	0.54
2:D:382:VAL:HG11	2:D:396:LEU:HD11	1.88	0.54
2:B:569:HIS:NE2	2:B:571:GLU:OE1	2.41	0.54
1:C:464:ASP:OD1	5:C:2502:HOH:O	2.18	0.54
1:C:906:ARG:HB3	1:C:928:GLU:HB2	1.90	0.54
1:A:1245:ILE:HG23	1:A:1336:LEU:HD22	1.90	0.53
2:D:206:THR:O	2:D:488:ARG:NH2	2.38	0.53
2:D:538:GLU:HB2	2:D:554:VAL:HB	1.91	0.53
2:D:664:PRO:HG2	2:D:690:MET:HG2	1.90	0.53
1:C:364:THR:O	5:C:2460:HOH:O	2.18	0.53
1:A:704:LYS:NZ	5:A:2344:HOH:O	2.39	0.53
2:B:381:GLU:OE1	2:B:611:TYR:OH	2.26	0.53
1:C:460:ALA:HB3	1:C:475:ILE:O	2.08	0.53
1:C:564:GLN:NE2	1:C:581:GLU:OE1	2.40	0.53
1:C:781:ASP:OD1	5:C:2353:HOH:O	2.19	0.53
1:A:553:VAL:HG22	1:A:554:SER:HB3	1.91	0.53
1:C:845:PHE:CG	1:C:906:ARG:HB2	2.44	0.53
2:D:154:VAL:HB	2:D:173:SER:HB2	1.90	0.53
1:C:1078:GLN:HG2	1:C:1147:TRP:CD2	2.44	0.53
1:A:392:MET:HB2	1:A:697:ARG:HG3	1.90	0.53
1:A:906:ARG:HB3	1:A:928:GLU:HB2	1.91	0.52
2:D:459:ASP:OD1	5:D:1066:HOH:O	2.19	0.52
1:A:1268:TRP:O	1:A:1330:ARG:HD3	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1033:ARG:NH1	5:A:2033:HOH:O	2.41	0.52
1:C:1332:PRO:HB2	1:C:1357:PHE:HD2	1.74	0.52
1:C:1003:GLN:NE2	5:C:2220:HOH:O	2.37	0.52
1:C:891:ASP:CG	1:C:936:ARG:HH12	2.17	0.52
1:C:236:LEU:HD21	1:C:239:ILE:HD11	1.92	0.52
1:A:1167:LYS:NZ	5:A:2427:HOH:O	2.40	0.51
1:C:174:LEU:HG	1:C:196:LEU:HA	1.92	0.51
1:C:670:GLN:HB3	1:C:687:THR:HB	1.92	0.51
1:C:777:HIS:ND1	5:C:1669:HOH:O	2.34	0.51
1:A:845:PHE:CG	1:A:906:ARG:HB2	2.46	0.51
1:A:900:TYR:CZ	1:A:936:ARG:HD2	2.45	0.51
1:C:709:ASN:HA	1:C:721:LEU:HB2	1.92	0.51
1:C:1219:ARG:HD2	1:C:1234:PRO:HD3	1.92	0.51
1:A:978:ASP:OD1	1:A:978:ASP:N	2.39	0.51
1:A:68:PHE:CE2	1:A:74:CYS:HB3	2.46	0.51
2:B:592:CYS:SG	5:B:827:HOH:O	2.59	0.51
1:A:357:VAL:HG22	1:A:374:LEU:HB3	1.93	0.51
1:A:492:TRP:HZ3	1:A:494:HIS:CE1	2.29	0.51
1:A:787:PHE:CZ	1:A:789:GLY:HA2	2.46	0.51
1:A:1095:GLN:HA	1:A:1098:VAL:HG23	1.91	0.51
2:D:630:LYS:HE2	2:D:633:ARG:HG2	1.93	0.50
2:B:279:LYS:NZ	5:B:899:HOH:O	2.31	0.50
2:D:337:ASP:OD1	2:D:341:ASN:N	2.42	0.50
2:D:563:ALA:N	5:D:1119:HOH:O	2.45	0.50
1:C:216:GLN:NE2	5:C:1984:HOH:O	2.37	0.50
1:C:787:PHE:CZ	1:C:789:GLY:HA2	2.46	0.50
1:A:181:ARG:NH1	5:A:1675:HOH:O	2.41	0.50
1:A:1388:ASN:ND2	1:A:1392:THR:HB	2.26	0.50
1:A:102:GLU:HG2	1:A:140:LEU:H	1.76	0.50
1:A:1437:ARG:NH1	5:A:1874:HOH:O	2.42	0.50
1:A:1473:VAL:HG23	2:B:15:PHE:HE2	1.77	0.50
1:A:120:ASN:OD1	1:A:120:ASN:N	2.44	0.50
2:D:309:GLN:OE1	5:D:1141:HOH:O	2.19	0.50
2:B:138:VAL:HB	2:B:151:GLU:HB2	1.93	0.50
1:C:1387:VAL:HG12	1:C:1393:PRO:HA	1.93	0.50
1:A:852:TRP:CZ2	1:A:859:GLY:HA3	2.47	0.50
1:C:1274:GLN:HG3	1:C:1288:TRP:CD1	2.47	0.50
2:D:27:TYR:OH	5:D:1098:HOH:O	2.13	0.50
2:D:402:ASP:OD1	2:D:404:SER:OG	2.23	0.50
2:B:202:ASN:O	2:B:208:ILE:HG12	2.13	0.49
1:A:221:ASP:OD2	5:A:2412:HOH:O	2.20	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:704:LYS:NZ	5:C:2113:HOH:O	2.45	0.49
2:B:154:VAL:HB	2:B:173:SER:HB2	1.94	0.49
1:A:855:ASP:OD2	1:A:953:ARG:HD2	2.12	0.49
1:C:1066:ALA:O	1:C:1082:ALA:N	2.43	0.49
1:C:1094:LEU:HD22	1:C:1106:ARG:HD2	1.94	0.49
1:C:1187:TYR:HA	1:C:1194:PRO:HA	1.95	0.49
1:C:357:VAL:HG22	1:C:374:LEU:HB3	1.94	0.49
1:C:497:PRO:HD2	1:C:525:LEU:HD21	1.94	0.49
1:C:730:TRP:CZ2	1:C:746:CYS:HB2	2.48	0.49
1:A:420:GLN:NE2	1:A:491:GLU:O	2.41	0.48
1:A:855:ASP:O	1:A:857:GLU:HA	2.13	0.48
1:A:640:LEU:HD23	1:A:684:LEU:HD13	1.94	0.48
1:C:273:GLU:O	1:C:289:THR:OG1	2.29	0.48
2:D:148:ARG:NH1	2:D:209:LEU:HB3	2.29	0.48
2:D:383:ALA:HB1	2:D:431:THR:HG21	1.96	0.48
2:D:566:ARG:NH2	2:D:632:VAL:HG21	2.29	0.48
2:B:428:ALA:HB3	2:B:433:ASN:HB3	1.95	0.48
1:C:1281:MET:HE3	1:C:1321:MET:HG2	1.96	0.48
1:C:1199:ASP:OD2	1:C:1203:ASN:HB2	2.14	0.48
2:B:81:THR:HB	2:B:89:THR:HG22	1.95	0.48
2:B:689:GLY:O	5:B:978:HOH:O	2.20	0.48
1:C:1378:GLN:NE2	1:C:1396:VAL:HG11	2.28	0.48
1:A:984:LEU:HD11	2:B:12:VAL:HG11	1.95	0.48
2:B:281:LEU:HD13	2:B:292:GLU:HB2	1.95	0.48
2:B:348:ASP:OD1	2:B:348:ASP:N	2.47	0.48
1:C:293:ALA:HB1	1:C:297:MET:CE	2.44	0.48
1:C:420:GLN:HG2	1:C:422:THR:O	2.14	0.48
1:C:961:VAL:HG11	1:C:1044:LEU:HD13	1.96	0.48
1:A:19:GLY:HA3	1:A:1356:LEU:HD12	1.96	0.47
1:C:942:GLN:HE21	2:D:17:ASN:HA	1.77	0.47
1:A:344:ASP:HB2	1:A:356:ALA:HB3	1.97	0.47
2:B:493:VAL:HB	2:B:501:ASP:HB2	1.95	0.47
2:B:184:ASP:HB2	2:B:194:SER:HB3	1.95	0.47
2:B:305:GLU:OE1	2:B:308:THR:OG1	2.30	0.47
2:D:374:LEU:O	2:D:415:TYR:OH	2.30	0.47
1:A:949:ILE:HG22	1:A:950:LYS:HG3	1.97	0.47
1:C:457:GLN:H	1:C:460:ALA:HB1	1.79	0.47
1:C:497:PRO:HD3	1:C:525:LEU:HD11	1.96	0.47
1:C:851:ARG:HG3	1:C:864:PHE:CE1	2.50	0.47
1:C:1181:LEU:HD21	2:D:169:GLY:HA3	1.97	0.47
2:D:158:ASN:O	2:D:163:LYS:HE2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:450:MET:HE1	2:D:474:GLN:HG2	1.96	0.47
2:D:649:PHE:CD2	2:D:690:MET:HG3	2.49	0.47
1:A:479:GLY:HA2	1:A:480:VAL:HA	1.61	0.47
1:A:1007:HIS:CE1	1:A:1017:GLY:H	2.33	0.47
1:C:404:TYR:OH	1:C:687:THR:OG1	2.27	0.46
2:D:428:ALA:HB3	2:D:433:ASN:HB3	1.97	0.46
2:D:479:LEU:HD22	2:D:487:LEU:HD11	1.97	0.46
1:A:1230:GLY:HA3	1:A:1343:TYR:CD2	2.50	0.46
1:A:460:ALA:HB2	1:A:476:THR:HG22	1.98	0.46
1:A:503:THR:OG1	1:A:504:GLU:OE1	2.34	0.46
1:C:1372:GLU:OE1	2:D:257:ASP:HB2	2.16	0.46
1:A:463:MET:SD	1:A:475:ILE:HD11	2.55	0.46
1:A:1274:GLN:HG3	1:A:1288:TRP:CD1	2.50	0.46
1:A:109:ASN:OD1	1:A:113:PHE:N	2.45	0.46
1:C:647:SER:HA	3:C:1504:GOL:H12	1.98	0.46
2:D:252:GLN:NE2	2:D:556:CYS:O	2.45	0.46
2:D:566:ARG:NH1	5:D:1111:HOH:O	2.48	0.46
1:A:391:GLU:O	1:A:393:PRO:HD3	2.15	0.46
2:D:552:LEU:HD13	2:D:570:TRP:CE2	2.51	0.46
1:A:243:ASN:HB3	1:A:263:TRP:CZ3	2.51	0.46
1:A:1188:ASP:OD1	1:A:1190:ARG:HG2	2.16	0.46
1:A:12:LEU:HD21	1:A:1172:VAL:HG23	1.98	0.45
1:A:219:CYS:HB2	1:A:224:ILE:HD11	1.97	0.45
1:A:1217:ALA:HA	1:A:1260:CYS:HA	1.99	0.45
1:A:521:SER:N	1:A:534:TYR:O	2.49	0.45
1:C:1067:TYR:HA	1:C:1081:VAL:HA	1.98	0.45
1:A:1186:ARG:HD2	1:A:1196:SER:HB3	1.98	0.45
1:A:1409:GLU:HA	5:A:1645:HOH:O	2.17	0.45
2:B:24:ASP:HB2	2:B:42:THR:HB	1.98	0.45
1:C:703:ASN:ND2	5:C:2338:HOH:O	2.36	0.45
2:D:556:CYS:HB3	2:D:564:GLN:NE2	2.31	0.45
2:B:599:ASP:HB3	2:B:605:ILE:HD11	1.99	0.45
1:A:934:TYR:CD1	1:A:941:PRO:HB3	2.51	0.45
1:A:964:ASN:HB2	1:A:997:HIS:HB2	1.99	0.45
1:A:1190:ARG:HG3	1:A:1191:PHE:CE2	2.52	0.45
1:C:102:GLU:OE2	1:C:876:ARG:NH2	2.47	0.45
1:A:1184:GLN:O	1:A:1197:LEU:HD12	2.17	0.45
1:C:993:GLN:HG2	2:D:16:ASP:HA	1.97	0.45
1:A:418:LEU:HD21	1:A:495:PHE:CD1	2.52	0.45
1:A:1199:ASP:OD2	1:A:1203:ASN:HB2	2.17	0.45
1:A:458:GLU:C	1:A:460:ALA:H	2.25	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1375:GLU:HG2	1:A:1395:LEU:HG	1.98	0.45
1:A:556:PRO:HD3	1:A:590:TRP:CZ2	2.52	0.45
2:D:69:SER:HB2	2:D:82:GLN:HB2	1.98	0.45
1:A:956:SER:HB3	1:A:1005:TYR:CE1	2.51	0.44
1:C:1007:HIS:CE1	1:C:1017:GLY:H	2.35	0.44
1:A:409:LEU:HD11	1:A:465:ILE:HD13	1.99	0.44
1:A:562:SER:OG	1:A:563:ARG:N	2.42	0.44
1:C:323:GLU:CD	1:C:328:ARG:HH21	2.25	0.44
1:C:1155:THR:OG1	2:D:96:GLU:OE1	2.29	0.44
1:C:1158:THR:HG22	2:D:133:GLY:HA3	1.99	0.44
1:C:1230:GLY:HA3	1:C:1343:TYR:CD2	2.52	0.44
2:D:566:ARG:HD3	2:D:566:ARG:HA	1.80	0.44
1:C:572:LEU:HD12	1:C:578:HIS:CE1	2.53	0.44
1:C:389:TRP:CD1	1:C:660:PRO:HD3	2.52	0.44
1:C:468:ASP:HB2	5:C:2502:HOH:O	2.17	0.44
2:D:296:ASN:CG	2:D:298:VAL:HG13	2.43	0.44
1:A:769:LEU:HB2	1:A:1412:GLY:HA3	1.99	0.44
1:C:353:THR:HB	1:C:378:TYR:CE1	2.52	0.44
2:D:680:ASN:HB3	2:D:684:LEU:HD13	2.00	0.44
1:C:59:TYR:HB2	1:C:72:TRP:CE2	2.53	0.44
1:C:977:PRO:C	1:C:979:ASP:H	2.25	0.44
2:D:381:GLU:OE1	2:D:611:TYR:OH	2.34	0.44
2:D:597:GLU:OE1	2:D:606:SER:OG	2.24	0.44
2:B:29:ARG:NH1	2:B:37:THR:OG1	2.48	0.44
1:C:293:ALA:HB1	1:C:297:MET:HE2	2.00	0.44
2:D:383:ALA:HA	2:D:384:GLY:HA2	1.72	0.44
1:A:240:ASP:HB3	1:A:263:TRP:CG	2.53	0.44
1:A:1341:ASP:OD1	1:A:1352:ARG:NH2	2.51	0.44
1:C:91:ASN:ND2	5:C:2207:HOH:O	2.48	0.44
1:C:908:GLN:HB2	1:C:927:ILE:HD13	2.00	0.44
1:C:1019:PRO:HB2	1:C:1065:VAL:HG21	1.99	0.44
2:D:148:ARG:NH1	2:D:210:ALA:O	2.50	0.44
2:D:261:GLN:NE2	5:D:841:HOH:O	2.50	0.44
2:D:331:ASP:HB3	2:D:348:ASP:HB2	2.00	0.44
2:D:316:THR:HB	2:D:330:GLN:HG2	1.98	0.43
2:D:610:TYR:O	3:D:701:GOL:H32	2.18	0.43
1:A:1382:ASP:O	1:A:1383:SER:OG	2.33	0.43
2:B:585:TRP:HZ3	2:B:600:GLY:HA2	1.83	0.43
1:C:1274:GLN:HA	1:C:1288:TRP:CD2	2.52	0.43
1:A:823:ILE:HA	1:A:824:PRO:HD3	1.87	0.43
1:A:891:ASP:CG	1:A:936:ARG:HH12	2.25	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:620:PHE:HB2	1:C:633:ILE:HB	2.00	0.43
1:C:1280:ARG:HH21	1:C:1320:LEU:HD23	1.83	0.43
2:D:387:GLN:HG3	2:D:435:TYR:CD2	2.53	0.43
2:B:421:LEU:HD21	2:B:424:ILE:HD11	2.00	0.43
1:C:236:LEU:O	1:C:271:TYR:OH	2.34	0.43
1:A:624:ILE:HD12	1:A:700:LEU:HD13	2.01	0.43
1:A:1483:ALA:HA	1:A:1484:ASN:HA	1.72	0.43
1:C:1184:GLN:O	1:C:1197:LEU:HD12	2.19	0.43
1:A:1352:ARG:HG2	2:B:258:ILE:O	2.19	0.43
1:C:192:ALA:HB1	1:C:303:PHE:CD1	2.54	0.43
1:C:1417:ILE:O	1:C:1444:THR:HA	2.19	0.43
1:C:462:LEU:HD21	1:C:506:PHE:CE2	2.54	0.43
1:C:1123:ARG:NH1	5:C:2453:HOH:O	2.51	0.43
1:A:414:THR:OG1	1:A:727:ALA:HB1	2.19	0.43
2:B:416:ASP:OD1	2:B:420:ASN:N	2.51	0.43
2:B:475:GLN:NE2	5:B:861:HOH:O	2.41	0.43
2:B:497:GLU:HA	2:B:498:THR:HA	1.74	0.43
2:D:496:GLY:C	2:D:498:THR:H	2.27	0.43
1:A:692:SER:HA	1:A:693:PRO:C	2.43	0.43
1:A:808:ILE:HG12	1:A:1417:ILE:HG23	2.00	0.43
2:B:233:THR:HG23	2:B:241:VAL:HG13	2.00	0.43
1:C:28:VAL:HG23	5:C:2451:HOH:O	2.18	0.43
2:D:511:SER:O	2:D:511:SER:OG	2.37	0.43
1:A:900:TYR:CE1	1:A:936:ARG:HD2	2.53	0.42
1:A:1007:HIS:O	5:A:2358:HOH:O	2.21	0.42
2:B:649:PHE:HD2	2:B:688:ASP:HB2	1.82	0.42
1:C:166:SER:HA	1:C:167:PRO:HD3	1.88	0.42
2:D:388:GLN:OE1	2:D:411:ARG:NH2	2.36	0.42
1:C:1116:GLN:NE2	5:C:2349:HOH:O	2.29	0.42
2:D:246:ASP:OD1	2:D:249:GLY:N	2.52	0.42
2:D:253:ARG:HD3	2:D:274:GLU:OE2	2.19	0.42
1:A:660:PRO:HG2	1:A:663:VAL:HG21	2.02	0.42
1:C:704:LYS:HG3	1:C:753:HIS:NE2	2.34	0.42
2:D:59:ARG:HB2	2:D:417:SER:HB2	2.00	0.42
2:B:333:ARG:HB2	2:B:346:THR:OG1	2.20	0.42
1:C:1000:LYS:NZ	5:C:1751:HOH:O	2.51	0.42
1:C:1352:ARG:HG2	2:D:258:ILE:O	2.19	0.42
1:C:1411:ASP:CB	1:C:1417:ILE:HD11	2.48	0.42
2:B:530:ARG:O	2:B:540:ARG:HA	2.19	0.42
1:C:17:GLY:N	5:C:2450:HOH:O	2.40	0.42
1:C:934:TYR:CD1	1:C:941:PRO:HB3	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:935:GLN:HB2	1:A:1470:PRO:HD3	2.02	0.42
1:C:1023:ARG:HE	1:C:1025:ASP:CG	2.28	0.42
1:C:402:GLN:HA	1:C:403:PRO:HD3	1.81	0.42
1:C:1123:ARG:HG3	1:C:1127:GLU:HB2	2.01	0.42
1:C:1388:ASN:HD21	1:C:1392:THR:HB	1.83	0.42
1:A:242:GLY:HA3	1:A:265:PHE:CD2	2.54	0.42
1:C:812:PRO:HG2	1:C:890:ASP:HB2	2.00	0.42
1:C:935:GLN:HB2	1:C:1470:PRO:HD3	2.02	0.42
1:C:1353:GLN:HB2	1:C:1370:ARG:HB2	2.02	0.42
1:A:512:LEU:O	1:A:516:VAL:HG22	2.20	0.42
1:A:1363:ARG:NH1	5:A:1688:HOH:O	2.50	0.42
1:C:68:PHE:CE2	1:C:74:CYS:HB3	2.55	0.42
1:C:953:ARG:NH1	5:C:2429:HOH:O	2.52	0.42
2:B:374:LEU:O	2:B:415:TYR:OH	2.32	0.42
1:A:1124:VAL:O	1:A:1127:GLU:HG3	2.20	0.41
1:C:1021:GLU:HB3	1:C:1121:LEU:HD13	2.02	0.41
1:A:1187:TYR:HA	1:A:1194:PRO:HA	2.02	0.41
2:B:227:GLU:CD	2:B:227:GLU:H	2.27	0.41
2:B:449:VAL:HB	2:B:453:LEU:HD12	2.02	0.41
1:C:840:GLN:HB2	1:C:968:ARG:NH1	2.35	0.41
1:C:1018:LEU:HD23	1:C:1018:LEU:HA	1.86	0.41
1:C:1274:GLN:HG2	5:C:2203:HOH:O	2.21	0.41
1:C:1345:SER:HA	3:C:1503:GOL:H2	2.02	0.41
1:C:1415:GLN:O	1:C:1417:ILE:HD12	2.19	0.41
1:A:748:LEU:HA	1:A:749:PRO:HD3	1.78	0.41
1:A:814:ARG:NH1	1:A:890:ASP:OD1	2.54	0.41
1:A:1089:LEU:HB2	1:A:1131:TRP:HB2	2.02	0.41
1:A:1220:PHE:O	1:A:1231:TYR:HB2	2.20	0.41
2:B:469:SER:HB3	2:B:481:TRP:CE2	2.55	0.41
2:B:563:ALA:N	2:B:566:ARG:HE	2.18	0.41
2:D:395:PRO:HA	2:D:619:TRP:O	2.21	0.41
2:D:407:THR:HG22	5:D:960:HOH:O	2.20	0.41
2:B:69:SER:HB2	2:B:82:GLN:HB2	2.03	0.41
2:B:569:HIS:ND1	2:B:581:ASP:OD1	2.36	0.41
2:D:80:TYR:CE2	2:D:82:GLN:HG3	2.56	0.41
1:A:146:LYS:NZ	1:A:148:GLU:OE2	2.50	0.41
2:B:92:LEU:HB3	2:B:101:ILE:HG22	2.02	0.41
1:C:1340:THR:HG22	1:C:1351:LEU:HD22	2.03	0.41
2:D:334:TYR:O	5:D:1126:HOH:O	2.21	0.41
2:D:676:MET:HG3	2:D:677:VAL:HG22	2.02	0.41
1:A:184:ASN:HB3	1:A:187:ASN:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:404:TYR:H	1:A:670:GLN:HE22	1.68	0.41
2:B:54:GLN:NE2	5:B:1030:HOH:O	2.53	0.41
2:B:388:GLN:OE1	2:B:411:ARG:NH2	2.24	0.41
2:B:127:GLU:O	2:B:133:GLY:HA2	2.20	0.41
1:C:59:TYR:HB2	1:C:72:TRP:CD2	2.56	0.41
2:D:614:GLY:HA2	2:D:634:TYR:CD1	2.56	0.41
1:A:14:LEU:HD23	1:A:14:LEU:HA	1.89	0.41
1:A:41:ILE:HD11	1:A:376:PHE:HZ	1.86	0.41
1:A:43:LEU:HD12	1:A:55:LEU:HB2	2.02	0.41
1:A:348:ASN:HB3	1:A:351:VAL:O	2.20	0.41
1:A:663:VAL:HG22	1:A:691:MET:HG2	2.03	0.41
1:A:1165:TRP:CE2	1:A:1172:VAL:HG12	2.55	0.41
1:A:1296:PHE:CE2	1:A:1308:ARG:HD3	2.56	0.41
1:A:1354:ARG:NH2	5:A:1988:HOH:O	2.53	0.41
1:C:145:ILE:HG22	1:C:167:PRO:HD3	2.02	0.41
1:C:633:ILE:HD13	1:C:684:LEU:HD21	2.03	0.41
1:C:876:ARG:O	1:C:879:LYS:HB2	2.21	0.41
1:A:257:LEU:HD23	1:A:257:LEU:HA	1.95	0.41
2:B:12:VAL:HB	2:B:25:ILE:HB	2.03	0.41
1:C:266:HIS:HB2	1:C:319:PHE:HB2	2.03	0.41
1:C:389:TRP:CG	1:C:660:PRO:HD3	2.56	0.41
2:D:469:SER:HB3	2:D:481:TRP:CE2	2.56	0.41
1:A:584:ALA:HB1	1:A:609:GLN:O	2.21	0.40
1:A:1296:PHE:CZ	1:A:1308:ARG:HD3	2.56	0.40
1:C:116:VAL:HG11	1:C:132:LYS:HE3	2.03	0.40
1:C:1417:ILE:HD12	1:C:1417:ILE:N	2.36	0.40
1:C:278:ILE:O	1:C:362:TYR:OH	2.34	0.40
1:C:1245:ILE:HG23	1:C:1336:LEU:HD22	2.02	0.40
1:C:1296:PHE:CE2	1:C:1308:ARG:HG3	2.56	0.40
1:A:391:GLU:O	5:A:2218:HOH:O	2.22	0.40
1:C:418:LEU:HD21	1:C:495:PHE:CD1	2.56	0.40
1:C:455:ARG:O	1:C:461:THR:HG21	2.21	0.40
1:C:1402:TRP:CE2	1:C:1428:TRP:HB3	2.57	0.40
1:A:1280[B]:ARG:HA	1:A:1280[B]:ARG:HD3	1.87	0.40
1:A:1312:MET:HE3	1:A:1312:MET:HB3	1.91	0.40
1:C:772:GLU:OE2	5:C:1739:HOH:O	2.21	0.40
1:C:964:ASN:HB2	1:C:997:HIS:HB2	2.03	0.40
1:C:1433:ASP:O	1:C:1437:ARG:HG3	2.21	0.40
1:A:452:LYS:O	1:A:454:PRO:HD3	2.22	0.40
1:A:579:LEU:HB3	1:A:590:TRP:HB2	2.04	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	1448/1488 (97%)	1395 (96%)	52 (4%)	1 (0%)	48	68
1	C	1441/1488 (97%)	1387 (96%)	54 (4%)	0	100	100
2	B	654/690 (95%)	628 (96%)	24 (4%)	2 (0%)	36	55
2	D	659/690 (96%)	627 (95%)	30 (5%)	2 (0%)	36	55
All	All	4202/4356 (96%)	4037 (96%)	160 (4%)	5 (0%)	48	68

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	564	GLN
2	D	498	THR
1	A	468	ASP
2	D	112	GLY
2	B	496	GLY

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	1198/1266 (95%)	1176 (98%)	22 (2%)	51	77
1	C	1194/1266 (94%)	1185 (99%)	9 (1%)	73	88
2	B	534/579 (92%)	526 (98%)	8 (2%)	57	80
2	D	536/579 (93%)	532 (99%)	4 (1%)	76	89
All	All	3462/3690 (94%)	3419 (99%)	43 (1%)	63	83

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	ILE
1	A	142	GLN
1	A	221	ASP
1	A	289	THR
1	A	317	LEU
1	A	336	VAL
1	A	391	GLU
1	A	435	ILE
1	A	447	MET
1	A	504	GLU
1	A	520	LEU
1	A	553	VAL
1	A	605	GLU
1	A	609	GLN
1	A	657	LEU
1	A	688	VAL
1	A	823	ILE
1	A	1181	LEU
1	A	1308	ARG
1	A	1331	THR
1	A	1417	ILE
1	A	1460	LYS
2	B	208	ILE
2	B	339	VAL
2	B	348	ASP
2	B	407	THR
2	B	514	ILE
2	B	564	GLN
2	B	574	LYS
2	B	579	ILE
1	C	256	GLU
1	C	336	VAL
1	C	357	VAL
1	C	421	GLU
1	C	609	GLN
1	C	823	ILE
1	C	1016	LEU
1	C	1081	VAL
1	C	1208	VAL
2	D	298	VAL
2	D	339	VAL
2	D	579	ILE

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Mol	Chain	Res	Type
2	D	690	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	89	GLN
1	A	216	GLN
1	A	229	GLN
1	A	326	ASN
1	A	670	GLN
1	A	672	GLN
1	A	946	GLN
1	A	995	GLN
1	A	997	HIS
1	A	1003	GLN
1	A	1022	GLN
1	A	1024	ASN
1	A	1366	GLN
2	B	62	HIS
2	B	125	GLN
2	B	261	GLN
2	B	275	GLN
2	B	373	GLN
2	B	387	GLN
2	B	474	GLN
2	B	679	ASN
2	B	680	ASN
1	C	89	GLN
1	C	630	ASN
1	C	753	HIS
1	C	1001	GLN
1	C	1022	GLN
1	C	1024	ASN
2	D	93	ASN
2	D	202	ASN
2	D	261	GLN
2	D	373	GLN
2	D	512	GLN
2	D	679	ASN
2	D	680	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 14 ligands modelled in this entry, 6 are monoatomic - leaving 8 for Mogul analysis.

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	GOL	C	1505	-	5,5,5	0.33	0	5,5,5	0.33	0
3	GOL	C	1502	-	5,5,5	0.37	0	5,5,5	0.37	0
3	GOL	A	1502	-	5,5,5	0.34	0	5,5,5	0.45	0
3	GOL	C	1503	-	5,5,5	0.35	0	5,5,5	0.31	0
3	GOL	D	701	-	5,5,5	0.36	0	5,5,5	0.19	0
3	GOL	C	1504	-	5,5,5	0.33	0	5,5,5	0.81	0
3	GOL	A	1501	-	5,5,5	0.35	0	5,5,5	0.26	0
3	GOL	C	1501	-	5,5,5	0.38	0	5,5,5	0.10	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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	C	1505	-	-	2/4/4/4	-
3	GOL	C	1502	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	A	1502	-	-	1/4/4/4	-
3	GOL	C	1503	-	-	2/4/4/4	-
3	GOL	D	701	-	-	2/4/4/4	-
3	GOL	C	1504	-	-	0/4/4/4	-
3	GOL	A	1501	-	-	3/4/4/4	-
3	GOL	C	1501	-	-	4/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1501	GOL	O1-C1-C2-C3
3	C	1501	GOL	O1-C1-C2-O2
3	C	1501	GOL	O1-C1-C2-C3
3	C	1502	GOL	O1-C1-C2-O2
3	C	1502	GOL	O1-C1-C2-C3
3	C	1501	GOL	C1-C2-C3-O3
3	C	1503	GOL	O1-C1-C2-C3
3	A	1501	GOL	O1-C1-C2-O2
3	C	1503	GOL	O1-C1-C2-O2
3	C	1501	GOL	O2-C2-C3-O3
3	D	701	GOL	C1-C2-C3-O3
3	C	1505	GOL	C1-C2-C3-O3
3	A	1501	GOL	C1-C2-C3-O3
3	A	1502	GOL	O2-C2-C3-O3
3	C	1505	GOL	O2-C2-C3-O3
3	D	701	GOL	O2-C2-C3-O3

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1502	GOL	1	0
3	C	1503	GOL	1	0
3	D	701	GOL	1	0
3	C	1504	GOL	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

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	1457/1488 (97%)	0.31	50 (3%)	48	43	24, 46, 69, 87	3 (0%)
1	C	1449/1488 (97%)	0.23	32 (2%)	62	58	25, 45, 66, 84	4 (0%)
2	B	666/690 (96%)	0.46	27 (4%)	41	37	40, 50, 66, 89	0
2	D	668/690 (96%)	0.40	29 (4%)	40	35	27, 50, 67, 95	1 (0%)
All	All	4240/4356 (97%)	0.32	138 (3%)	49	45	24, 47, 67, 95	8 (0%)

All (138) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	522	THR	5.0
2	D	498	THR	4.5
2	D	499	ALA	4.4
1	C	459	GLY	4.3
2	B	549	ALA	4.3
1	A	399	ASN	4.3
1	C	856	SER	4.2
2	D	522	THR	4.2
2	B	689	GLY	4.1
1	A	690	HIS	4.1
1	A	492	TRP	4.0
1	C	7	MET	4.0
2	B	383	ALA	4.0
2	D	349	ALA	3.9
1	A	856	SER	3.9
2	B	498	THR	3.9
2	D	523	ASN	3.9
1	A	553	VAL	3.8
1	C	492	TRP	3.8
2	B	111	ASN	3.8
1	C	536	ASN	3.7

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Mol	Chain	Res	Type	RSRZ
2	D	547	ALA	3.6
2	B	349	ALA	3.6
1	A	858	ALA	3.5
2	D	559	GLU	3.4
2	B	112	GLY	3.4
2	D	524	HIS	3.4
2	D	111	ASN	3.3
1	A	491	GLU	3.3
2	D	689	GLY	3.3
1	A	422	THR	3.3
1	A	466	ASN	3.3
2	B	4	GLN	3.2
2	B	110	GLU	3.2
1	A	1389	VAL	3.2
1	C	399	ASN	3.1
1	A	480	VAL	3.1
2	B	687	PRO	3.1
2	D	690	MET	3.0
1	A	1484	ASN	3.0
2	D	215	ASN	3.0
2	B	525	SER	3.0
2	B	361	VAL	3.0
1	A	661	ASP	3.0
1	A	537	GLN	3.0
1	A	458	GLU	2.9
1	C	460	ALA	2.9
2	D	496	GLY	2.9
1	C	728[A]	GLN	2.9
1	A	479	GLY	2.9
1	A	468	ASP	2.8
1	A	855	ASP	2.8
2	D	494	ALA	2.8
1	A	8	ALA	2.8
1	A	459	GLY	2.7
1	C	9	ILE	2.7
2	D	548	GLU	2.7
2	D	500	ASP	2.7
2	D	544	GLY	2.7
1	C	1389	VAL	2.7
2	B	563	ALA	2.7
1	A	857	GLU	2.7
2	D	688	ASP	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	467	GLY	2.7
1	A	562	SER	2.7
1	A	401	TYR	2.6
2	D	549	ALA	2.6
1	A	1483	ALA	2.6
2	D	362	PRO	2.6
1	A	456	LEU	2.6
2	B	515	LEU	2.5
1	A	536	ASN	2.5
2	B	518	SER	2.5
1	C	400	GLY	2.5
2	D	687	PRO	2.4
1	C	857	GLU	2.4
1	C	811	HIS	2.4
1	A	423	PRO	2.4
1	A	1377	TRP	2.4
2	D	383	ALA	2.4
2	B	362	PRO	2.4
2	D	64	GLU	2.4
1	A	420	GLN	2.4
1	C	456	LEU	2.3
2	D	521	GLN	2.3
1	C	401	TYR	2.3
1	A	518	ALA	2.3
1	A	517	GLY	2.3
1	C	561	ASP	2.3
2	B	384	GLY	2.3
1	C	1377	TRP	2.3
2	B	5	LEU	2.3
1	A	1054	ASN	2.2
2	B	430	ALA	2.2
1	A	403	PRO	2.2
1	C	455	ARG	2.2
1	A	535	ALA	2.2
1	C	8	ALA	2.2
2	B	62	HIS	2.2
1	A	7	MET	2.2
1	A	688	VAL	2.2
1	C	425	ALA	2.2
2	D	563	ALA	2.2
2	B	385	ALA	2.2
1	C	454	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	549	GLN	2.1
1	A	288	THR	2.1
1	A	1391	GLY	2.1
1	C	453	ILE	2.1
1	C	1126	SER	2.1
2	D	216	ASP	2.1
1	A	460	ALA	2.1
2	D	144	GLY	2.1
1	A	1123	ARG	2.1
2	B	386	GLY	2.1
2	B	407	THR	2.1
1	A	563	ARG	2.1
1	A	435	ILE	2.1
1	A	453	ILE	2.1
1	A	693	PRO	2.1
1	A	398	PHE	2.1
1	A	670	GLN	2.1
1	A	425	ALA	2.1
1	A	478	ALA	2.1
1	C	1483	ALA	2.1
1	C	1054	ASN	2.1
1	C	662	GLY	2.1
2	D	108	ARG	2.1
2	B	227	GLU	2.1
1	C	457	GLN	2.0
2	B	432	ASN	2.0
2	D	685	THR	2.0
1	C	562	SER	2.0
1	A	665	PHE	2.0
1	C	17	GLY	2.0
2	B	544	GLY	2.0
1	C	472	ASP	2.0
1	C	1390	SER	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	GOL	C	1503	6/6	0.81	0.15	59,61,62,62	0
3	GOL	C	1501	6/6	0.82	0.14	55,56,58,60	0
3	GOL	C	1504	6/6	0.82	0.17	43,46,48,51	0
3	GOL	C	1502	6/6	0.87	0.18	47,48,51,53	0
3	GOL	C	1505	6/6	0.87	0.14	50,52,55,56	0
3	GOL	A	1502	6/6	0.89	0.15	46,47,49,49	0
3	GOL	A	1501	6/6	0.90	0.12	49,50,51,52	0
3	GOL	D	701	6/6	0.90	0.14	48,50,52,52	0
4	K	C	1508	1/1	0.91	0.12	56,56,56,56	0
4	K	A	1505	1/1	0.92	0.13	57,57,57,57	0
4	K	A	1503	1/1	0.98	0.03	45,45,45,45	0
4	K	C	1506	1/1	0.99	0.04	39,39,39,39	0
4	K	C	1507	1/1	0.99	0.05	50,50,50,50	0
4	K	A	1504	1/1	0.99	0.10	49,49,49,49	0

6.5 Other polymers [i](#)

There are no such residues in this entry.