



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 09:16 AM GMT

PDB ID : 3HRZ
Title : Cobra Venom Factor (CVF) in complex with human factor B
Authors : Janssen, B.J.C.; Gomes, L.; Koning, R.I.; Svergun, D.I.; Koster, A.J.;
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Deposited on : 2009-06-10
Resolution : 2.20 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

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

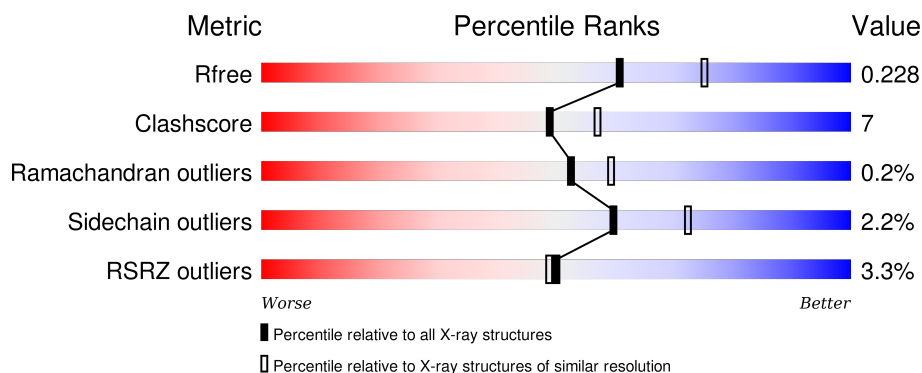
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	3774 (2.20-2.20)
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (2.20-2.20)

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 $\leq 5\%$. 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	627	<div> <div>86%</div> <div>11% ..</div> </div>
2	B	252	<div> <div>77%</div> <div>13% • 8%</div> </div>
3	C	379	<div> <div>78%</div> <div>17% • •</div> </div>
4	D	741	<div> <div>75%</div> <div>18% 6%</div> </div>

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
10	NAG	D	9097	-	-	-	X
5	NAG	A	9187	-	-	-	X
5	NAG	C	9324	X	-	-	X
8	P6G	A	630	-	-	-	X
9	PO4	D	745	-	-	-	X

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 15938 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 Cobra venom factor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	614	Total	C	N	O	S	0	0	0
			4800	3071	804	910	15			

- Molecule 2 is a protein called Cobra venom factor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	233	Total	C	N	O	S	0	0	0
			1856	1194	311	346	5			

- Molecule 3 is a protein called Cobra venom factor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	362	Total	C	N	O	S	0	0	0
			2926	1847	490	570	19			

- Molecule 4 is a protein called Complement factor B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	693	Total	C	N	O	S	0	0	0
			5469	3449	947	1040	33			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	254	GLY	ASP	ENGINEERED	UNP P00751
D	260	ASP	ASN	ENGINEERED	UNP P00751
D	740	ALA	-	INSERTION	UNP P00751
D	741	ALA	-	INSERTION	UNP P00751

- Molecule 5 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: C₈H₁₅NO₆).



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

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Mg	0	0
			1	1		
6	D	1	Total	Mg	0	0
			1	1		

- Molecule 7 is POTASSIUM ION (three-letter code: K) (formula: K).

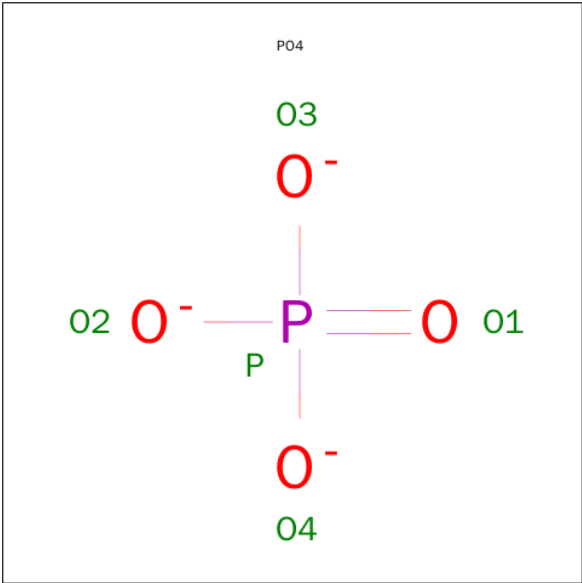
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	K	0	0
			1	1		

- Molecule 8 is HEXAETHYLENE GLYCOL (three-letter code: P6G) (formula: C₁₂H₂₆O₇).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			19	12	7		
8	C	1	Total	C	O	0	0
			19	12	7		

- Molecule 9 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	B	1	Total	O	P	0	0
			5	4	1		
9	C	1	Total	O	P	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	D	1	Total	O	P	0	0
			5	4	1		
9	D	1	Total	O	P	0	0
			5	4	1		
9	D	1	Total	O	P	0	0
			5	4	1		

- Molecule 10 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	D	2	Total	C	N	O	0	0
			28	16	2	10		

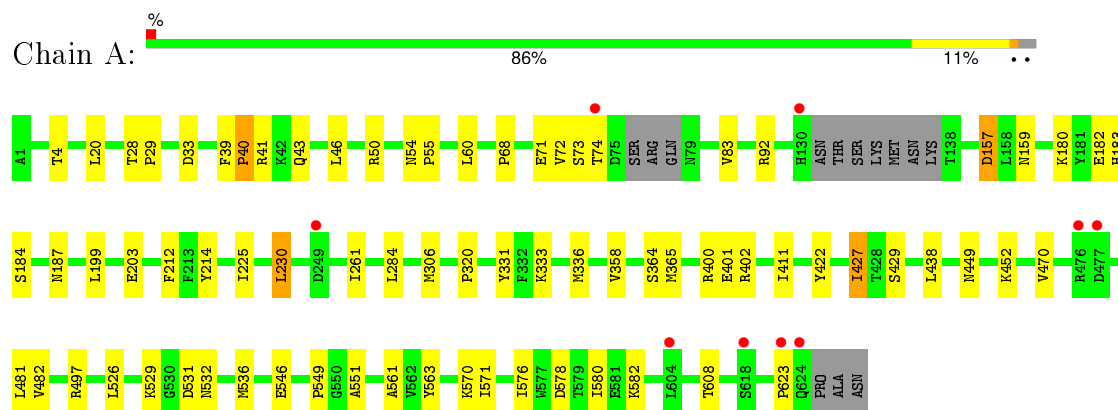
- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	290	Total	O	0	0
			290	290		
11	B	100	Total	O	0	0
			100	100		
11	C	129	Total	O	0	0
			129	129		
11	D	232	Total	O	0	0
			232	232		


3 Residue-property plots

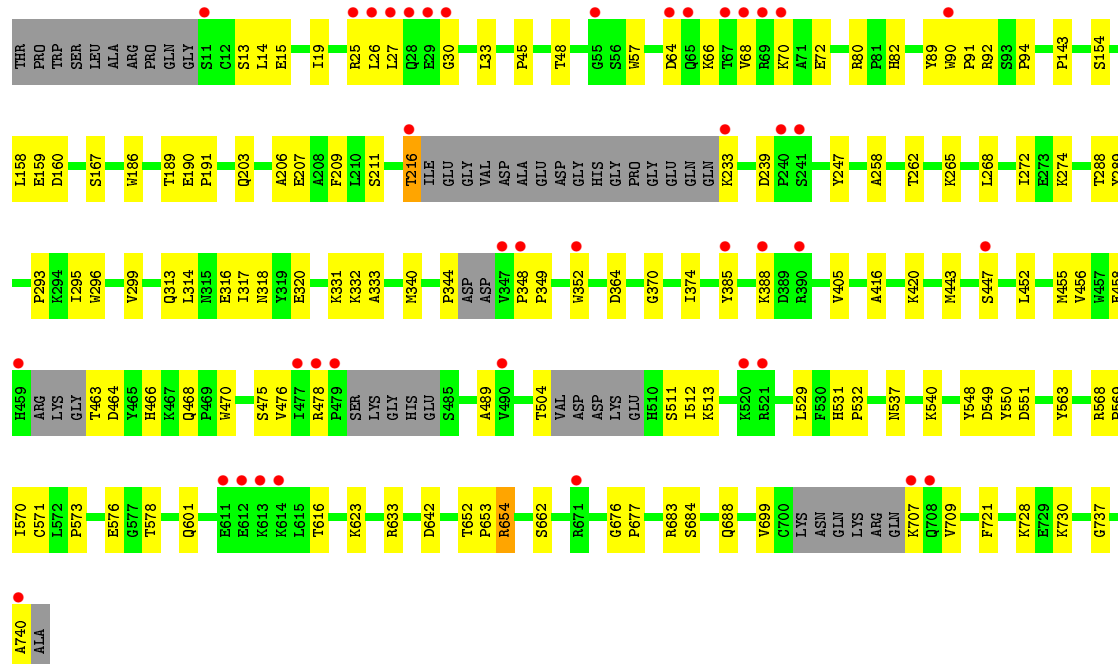
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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



● Molecule 4: Complement factor B

Chain D:  6% 75% 18% 6%



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	128.89Å 283.39Å 134.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	33.49 – 2.20 33.49 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.5 (33.49-2.20) 99.5 (33.49-2.20)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.39 (at 2.20Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.180 , 0.226 0.182 , 0.228	Depositor DCC
R_{free} test set	2485 reflections (2.05%)	DCC
Wilson B-factor (Å ²)	32.9	Xtriage
Anisotropy	0.488	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 42.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 123930 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	15938	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.24% 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, 0.375 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: PO4, MG, K, NAG, P6G

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	0.41	0/4908	0.56	1/6678 (0.0%)
2	B	0.38	0/1894	0.57	0/2570
3	C	0.38	0/2977	0.59	0/4026
4	D	0.35	0/5591	0.51	0/7567
All	All	0.38	0/15370	0.55	1/20841 (0.0%)

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
2	B	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	230	LEU	CA-CB-CG	-5.15	103.45	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	929	ASP	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4800	0	4797	51	0
2	B	1856	0	1900	34	0
3	C	2926	0	2873	49	0
4	D	5469	0	5339	94	1
5	A	14	0	13	3	0
5	C	14	0	13	0	0
5	D	14	0	13	0	0
6	A	1	0	0	0	0
6	D	1	0	0	0	0
7	A	1	0	0	0	0
8	A	19	0	26	3	0
8	C	19	0	26	4	0
9	B	5	0	0	0	0
9	C	5	0	0	0	0
9	D	15	0	0	0	0
10	D	28	0	25	2	0
11	A	290	0	0	0	0
11	B	100	0	0	2	0
11	C	129	0	0	2	1
11	D	232	0	0	7	0
All	All	15938	0	15025	217	1

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 7.

All (217) 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)
8:A:630:P6G:H91	8:A:630:P6G:C15	2.03	0.88
4:D:64:ASP:HB2	4:D:66:LYS:HG3	1.60	0.83
3:C:1445:LYS:HD3	8:C:100:P6G:H182	1.62	0.81
4:D:699:VAL:HG21	4:D:709:VAL:HG22	1.62	0.80
8:A:630:P6G:H91	8:A:630:P6G:H151	1.64	0.80
4:D:475:SER:HB3	4:D:513:LYS:HE3	1.62	0.79
2:B:943:ILE:HD11	3:C:1301:MET:CE	2.16	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:728:LYS:HE3	4:D:740:ALA:HB3	1.67	0.75
2:B:943:ILE:HD11	3:C:1301:MET:HE2	1.67	0.74
1:A:41:ARG:HH11	1:A:43:GLN:HG3	1.53	0.73
1:A:230:LEU:HD13	1:A:561:ALA:HB2	1.71	0.72
4:D:258:ALA:O	4:D:262:THR:HG23	1.89	0.71
4:D:529:LEU:HD13	4:D:730:LYS:HD2	1.73	0.70
3:C:1369:LEU:HB2	3:C:1395:MET:HE1	1.74	0.69
3:C:1251:LEU:HD13	3:C:1297:GLY:HA3	1.74	0.69
4:D:209:PHE:HD2	4:D:443:MET:HE1	1.58	0.69
2:B:861:VAL:H	3:C:1430:GLN:NE2	1.90	0.69
2:B:818:VAL:HG12	2:B:820:GLU:HG2	1.75	0.68
4:D:489:ALA:HB2	4:D:677:PRO:HG3	1.76	0.68
4:D:299:VAL:HG13	4:D:340:MET:CE	2.24	0.68
3:C:1261:ASP:HB3	3:C:1285:LEU:HD12	1.75	0.68
1:A:429:SER:HB2	1:A:438:LEU:CD1	2.24	0.68
4:D:478:ARG:HH12	4:D:504:THR:HG22	1.60	0.67
8:A:630:P6G:H91	8:A:630:P6G:H152	1.74	0.67
4:D:299:VAL:HG13	4:D:340:MET:HE3	1.77	0.67
1:A:551:ALA:HA	2:B:773:THR:HG23	1.76	0.67
4:D:26:LEU:HD22	4:D:30:GLY:HA2	1.79	0.65
3:C:1619:PRO:HD2	11:C:484:HOH:O	1.96	0.65
4:D:550:TYR:CZ	4:D:654:ARG:HD3	2.32	0.65
4:D:475:SER:O	4:D:513:LYS:HG3	1.97	0.64
3:C:1571:THR:HG21	3:C:1576:SER:OG	1.98	0.64
1:A:187:ASN:HD22	5:A:9187:NAG:H83	1.63	0.64
1:A:72:VAL:O	1:A:72:VAL:HG22	1.98	0.64
1:A:33:ASP:OD1	1:A:50:ARG:HD2	1.98	0.64
3:C:1422:LYS:HD3	3:C:1425:GLU:HG3	1.79	0.64
3:C:1369:LEU:HB2	3:C:1395:MET:CE	2.27	0.63
4:D:623:LYS:HE3	4:D:662:SER:O	1.99	0.62
4:D:233:LYS:HB3	4:D:233:LYS:NZ	2.14	0.61
4:D:374:ILE:HD11	4:D:416:ALA:HB1	1.82	0.61
4:D:549:ASP:OD1	4:D:654:ARG:HD2	2.01	0.61
3:C:1382:VAL:O	3:C:1382:VAL:HG12	2.00	0.61
2:B:898:VAL:HG21	3:C:1311:LEU:HD13	1.83	0.61
4:D:385:TYR:CD1	4:D:388:LYS:HD3	2.36	0.60
4:D:452:LEU:HD23	4:D:455:MET:HG3	1.84	0.59
3:C:1573:ASP:O	3:C:1574:LYS:HG2	2.01	0.59
3:C:1469:ARG:HG3	3:C:1578:ILE:HD11	1.83	0.59
2:B:798:MET:HE1	2:B:872:VAL:HB	1.83	0.59
4:D:206:ALA:HA	4:D:443:MET:HE2	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:1330:ILE:HD13	3:C:1342:MET:HB2	1.85	0.59
4:D:203:GLN:HB3	4:D:458:GLU:HG3	1.85	0.59
1:A:333:LYS:HB3	1:A:336:MET:HE3	1.86	0.58
4:D:265:LYS:HE3	4:D:314:LEU:O	2.03	0.58
4:D:296:TRP:CE2	4:D:317:ILE:HD12	2.38	0.58
4:D:563:TYR:CZ	4:D:569:PRO:HG3	2.38	0.58
1:A:20:LEU:HD13	1:A:470:VAL:HG11	1.85	0.57
4:D:677:PRO:HD2	11:D:795:HOH:O	2.05	0.57
2:B:926:ARG:HD2	3:C:1305:THR:OG1	2.04	0.57
4:D:14:LEU:HD21	4:D:26:LEU:HD11	1.87	0.56
4:D:288:THR:HG21	4:D:317:ILE:HG21	1.85	0.56
4:D:299:VAL:H	4:D:340:MET:HE3	1.70	0.56
1:A:41:ARG:NH1	1:A:43:GLN:HG3	2.21	0.56
1:A:449:ASN:HA	1:A:452:LYS:HE3	1.88	0.56
4:D:683:ARG:O	4:D:684:SER:HB2	2.05	0.56
3:C:1261:ASP:HB3	3:C:1285:LEU:CD1	2.36	0.56
3:C:1426:VAL:HG23	3:C:1429:ILE:HD13	1.88	0.56
4:D:570:ILE:HD13	4:D:688:GLN:HB2	1.88	0.55
1:A:549:PRO:HG3	2:B:744:PRO:HG3	1.88	0.55
4:D:364:ASP:HB3	4:D:405:VAL:O	2.07	0.55
2:B:869:LEU:HD23	2:B:892:LYS:HA	1.89	0.54
1:A:529:LYS:HE3	1:A:546:GLU:OE2	2.07	0.54
4:D:143:PRO:HG3	4:D:186:TRP:CZ2	2.42	0.54
2:B:898:VAL:CG2	3:C:1311:LEU:HD13	2.37	0.54
1:A:54:ASN:HB2	1:A:55:PRO:HD2	1.90	0.54
4:D:64:ASP:HB2	4:D:66:LYS:CG	2.37	0.53
4:D:216:THR:HG22	11:D:908:HOH:O	2.08	0.53
1:A:214:TYR:CE1	1:A:402:ARG:HD2	2.43	0.53
4:D:699:VAL:HG22	4:D:699:VAL:O	2.09	0.53
1:A:358:VAL:HG12	1:A:365:MET:HG2	1.91	0.53
4:D:478:ARG:HH12	4:D:504:THR:CG2	2.22	0.52
4:D:313:GLN:O	4:D:316:GLU:HB2	2.09	0.52
2:B:798:MET:HE2	2:B:889:LYS:HB2	1.91	0.52
4:D:80:ARG:HD3	4:D:94:PRO:O	2.10	0.52
3:C:1481:GLN:NE2	11:C:730:HOH:O	2.43	0.52
3:C:1253:LEU:HD13	3:C:1255:ILE:HD11	1.91	0.52
1:A:306:MET:HB3	8:C:100:P6G:H51	1.90	0.52
4:D:344:PRO:HB2	11:D:972:HOH:O	2.09	0.52
1:A:4:THR:HG22	1:A:608:THR:HG22	1.92	0.52
3:C:1462:ILE:HD13	3:C:1542:ILE:HG22	1.92	0.52
2:B:818:VAL:CG1	2:B:820:GLU:HG2	2.38	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:207:GLU:O	4:D:211:SER:HB3	2.10	0.51
2:B:943:ILE:HD11	3:C:1301:MET:HE3	1.92	0.51
3:C:1251:LEU:CD1	3:C:1297:GLY:HA3	2.40	0.51
4:D:550:TYR:CE2	4:D:654:ARG:HD3	2.45	0.51
10:D:9097:NAG:O4	10:D:9098:NAG:H61	2.11	0.51
4:D:571:CYS:HB3	4:D:578:THR:OG1	2.11	0.51
1:A:497:ARG:HG3	1:A:497:ARG:HH11	1.76	0.51
3:C:1464:ILE:HD11	3:C:1569:LEU:HD13	1.92	0.50
1:A:576:ILE:O	1:A:580:ILE:HG12	2.11	0.50
4:D:676:GLY:HA3	11:D:928:HOH:O	2.11	0.50
3:C:1486:VAL:O	3:C:1490:ILE:HG12	2.12	0.50
3:C:1382:VAL:O	3:C:1382:VAL:CG1	2.60	0.50
1:A:180:LYS:NZ	5:A:9187:NAG:H81	2.26	0.50
3:C:1442:LEU:O	8:C:100:P6G:H152	2.11	0.49
4:D:274:LYS:HE3	4:D:443:MET:O	2.12	0.49
4:D:388:LYS:HG2	11:D:807:HOH:O	2.11	0.49
4:D:33:LEU:O	4:D:33:LEU:HD12	2.12	0.49
4:D:247:TYR:CD1	4:D:340:MET:HE1	2.48	0.49
3:C:1571:THR:HG23	3:C:1571:THR:O	2.13	0.49
4:D:233:LYS:HZ3	4:D:233:LYS:HB3	1.76	0.49
4:D:45:PRO:HG3	4:D:68:VAL:HG21	1.95	0.49
3:C:1268:TYR:OH	3:C:1281:VAL:HG23	2.13	0.48
1:A:39:PHE:CD1	1:A:40:PRO:HA	2.49	0.48
3:C:1395:MET:HE1	3:C:1423:HIS:HB2	1.96	0.47
1:A:578:ASP:O	1:A:582:LYS:HG2	2.13	0.47
4:D:314:LEU:O	4:D:317:ILE:HG12	2.14	0.47
3:C:1516:ASP:OD2	3:C:1548:GLN:HG2	2.15	0.47
4:D:299:VAL:HG22	4:D:340:MET:HE2	1.96	0.47
1:A:333:LYS:CB	1:A:336:MET:HE3	2.44	0.47
1:A:427:ILE:CG2	1:A:438:LEU:HD11	2.45	0.47
2:B:819:ASN:HA	2:B:853:LEU:HG	1.97	0.47
1:A:199:LEU:HD11	2:B:731:LYS:HG2	1.97	0.47
4:D:548:TYR:O	4:D:551:ASP:HB2	2.15	0.46
4:D:143:PRO:HG3	4:D:186:TRP:CE2	2.50	0.46
1:A:333:LYS:HB3	1:A:336:MET:CE	2.45	0.46
3:C:1285:LEU:HD13	3:C:1287:GLN:OE1	2.15	0.46
4:D:463:THR:HB	4:D:466:HIS:HB2	1.97	0.46
4:D:316:GLU:HA	4:D:316:GLU:OE1	2.16	0.46
1:A:570:LYS:HG2	1:A:571:ILE:O	2.16	0.46
1:A:68:PRO:HB2	1:A:71:GLU:HG2	1.97	0.46
1:A:83:VAL:HG13	1:A:83:VAL:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:563:TYR:OH	2:B:768:LEU:HD11	2.16	0.46
3:C:1264:VAL:HA	3:C:1265:PRO:HD2	1.87	0.46
1:A:331:TYR:HA	1:A:411:ILE:O	2.16	0.46
3:C:1464:ILE:HD13	3:C:1569:LEU:HD22	1.97	0.45
4:D:89:TYR:CE2	4:D:92:ARG:HG2	2.51	0.45
1:A:182:GLU:O	1:A:183:HIS:HB2	2.15	0.45
4:D:537:ASN:HB3	4:D:540:LYS:HD3	1.96	0.45
4:D:318:ASN:OD1	4:D:320:GLU:HG2	2.17	0.45
4:D:348:PRO:HB2	4:D:352:TRP:CD1	2.52	0.45
1:A:212:PHE:CZ	1:A:320:PRO:HB3	2.52	0.45
4:D:25:ARG:NH2	4:D:27:LEU:HD21	2.31	0.45
4:D:730:LYS:HA	4:D:730:LYS:HD3	1.77	0.45
1:A:481:LEU:HD23	1:A:482:VAL:N	2.32	0.45
1:A:157:ASP:OD2	1:A:159:ASN:HB2	2.17	0.45
1:A:333:LYS:N	1:A:333:LYS:HD2	2.31	0.45
4:D:652:THR:HB	4:D:653:PRO:CD	2.47	0.45
1:A:336:MET:HE2	1:A:422:TYR:HB2	1.99	0.45
2:B:720:ASP:CG	2:B:843:ARG:HH12	2.21	0.45
4:D:209:PHE:HD2	4:D:443:MET:CE	2.27	0.44
4:D:26:LEU:HD21	4:D:57:TRP:CZ2	2.52	0.44
2:B:851:LYS:HE3	2:B:851:LYS:HB3	1.87	0.44
3:C:1361:ASP:HB3	3:C:1435:LYS:HB2	1.99	0.44
2:B:766:VAL:CG1	2:B:783:PRO:HB3	2.47	0.44
2:B:860:PHE:HA	3:C:1430:GLN:HE22	1.82	0.44
4:D:158:LEU:O	4:D:159:GLU:HB2	2.18	0.44
1:A:429:SER:HB2	1:A:438:LEU:HD12	1.97	0.44
2:B:929:ASP:C	2:B:931:ARG:H	2.21	0.44
3:C:1384:ARG:HG2	3:C:1405:LEU:HD12	1.98	0.44
1:A:225:ILE:HD12	1:A:261:ILE:HD11	2.00	0.43
4:D:207:GLU:HA	4:D:207:GLU:OE1	2.18	0.43
1:A:73:SER:HB2	1:A:183:HIS:NE2	2.33	0.43
4:D:19:ILE:HG13	4:D:72:GLU:HA	2.00	0.43
4:D:476:VAL:HG22	4:D:512:ILE:HG23	2.00	0.43
4:D:573:PRO:HB3	4:D:721:PHE:CZ	2.54	0.43
4:D:331:LYS:HD3	4:D:370:GLY:O	2.17	0.43
10:D:9098:NAG:O3	10:D:9098:NAG:C7	2.66	0.43
3:C:1537:LYS:HA	3:C:1537:LYS:HD2	1.82	0.43
3:C:1569:LEU:HD11	3:C:1578:ILE:HG12	2.00	0.43
1:A:39:PHE:CG	1:A:40:PRO:HA	2.54	0.43
4:D:289:TYR:CG	4:D:333:ALA:HB2	2.54	0.43
4:D:463:THR:HG22	4:D:464:ASP:N	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:1284:LYS:HE2	4:D:160:ASP:OD1	2.19	0.43
1:A:28:THR:HA	1:A:29:PRO:HD3	1.89	0.43
2:B:926:ARG:NH1	3:C:1287:GLN:O	2.52	0.43
1:A:180:LYS:HZ1	5:A:9187:NAG:H81	1.84	0.43
4:D:268:LEU:O	4:D:272:ILE:HG12	2.18	0.43
4:D:652:THR:HB	4:D:653:PRO:HD2	2.00	0.42
4:D:295:ILE:HD12	4:D:295:ILE:N	2.33	0.42
4:D:190:GLU:HA	4:D:191:PRO:HD3	1.81	0.42
2:B:825:ARG:O	2:B:876:ALA:HA	2.18	0.42
3:C:1510:GLU:HB2	3:C:1517:ILE:HB	2.02	0.42
4:D:470:TRP:HA	4:D:568:ARG:O	2.19	0.42
4:D:33:LEU:C	4:D:33:LEU:HD12	2.40	0.42
2:B:816:ASN:O	2:B:853:LEU:HA	2.20	0.42
2:B:768:LEU:HB3	11:B:964:HOH:O	2.19	0.42
3:C:1360:ILE:HD13	3:C:1436:VAL:HG22	2.02	0.42
1:A:60:LEU:C	1:A:60:LEU:HD23	2.39	0.42
2:B:846:GLN:HG3	11:B:272:HOH:O	2.20	0.42
2:B:824:VAL:O	2:B:847:GLN:HA	2.20	0.42
4:D:13:SER:OG	4:D:15:GLU:HG3	2.20	0.42
2:B:915:VAL:HB	2:B:916:GLY:H	1.72	0.41
2:B:742:GLU:OE2	2:B:752:LYS:HD2	2.19	0.41
4:D:70:LYS:HD2	4:D:70:LYS:HA	1.79	0.41
3:C:1349:TYR:CG	3:C:1355:SER:HB3	2.55	0.41
2:B:923:ILE:N	2:B:923:ILE:HD12	2.35	0.41
4:D:730:LYS:HE3	11:D:938:HOH:O	2.20	0.41
3:C:1484:ILE:HB	3:C:1605:ASP:HB3	2.01	0.41
3:C:1405:LEU:HD23	3:C:1408:VAL:CG2	2.51	0.41
1:A:549:PRO:CG	2:B:744:PRO:HG3	2.51	0.41
1:A:214:TYR:OH	1:A:320:PRO:HG3	2.21	0.41
3:C:1517:ILE:HD13	3:C:1542:ILE:HG12	2.03	0.41
1:A:401:GLU:HG2	1:A:401:GLU:H	1.62	0.41
4:D:576:GLU:HG3	4:D:737:GLY:O	2.20	0.41
4:D:189:THR:HG22	4:D:420:LYS:HB3	2.03	0.41
4:D:274:LYS:HE2	4:D:447:SER:OG	2.21	0.41
1:A:180:LYS:HE3	1:A:184:SER:O	2.20	0.41
4:D:531:HIS:CG	4:D:532:PRO:HD2	2.56	0.41
4:D:468:GLN:HE21	4:D:468:GLN:HB2	1.76	0.41
1:A:526:LEU:HD22	2:B:771:SER:HB3	2.02	0.41
1:A:531:ASP:O	1:A:532:ASN:HB2	2.21	0.41
4:D:274:LYS:HA	4:D:274:LYS:HD2	1.84	0.41
2:B:757:TYR:HB3	4:D:92:ARG:HD3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:90:TRP:HA	4:D:91:PRO:HA	1.93	0.40
8:C:100:P6G:H81	8:C:100:P6G:H52	1.37	0.40
4:D:348:PRO:HA	4:D:349:PRO:HD3	1.90	0.40
4:D:456:VAL:CG2	4:D:470:TRP:HZ3	2.35	0.40
4:D:332:LYS:HE3	11:D:788:HOH:O	2.20	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:633:ARG:NH1	11:C:574:HOH:O[3_455]	2.19	0.01

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	608/627 (97%)	597 (98%)	9 (2%)	2 (0%)	46	50
2	B	231/252 (92%)	223 (96%)	8 (4%)	0	100	100
3	C	356/379 (94%)	345 (97%)	10 (3%)	1 (0%)	46	50
4	D	679/741 (92%)	653 (96%)	26 (4%)	0	100	100
All	All	1874/1999 (94%)	1818 (97%)	53 (3%)	3 (0%)	52	59

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	1318	CYS
1	A	74	THR
1	A	623	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	536/548 (98%)	526 (98%)	10 (2%)	65	77
2	B	210/227 (92%)	207 (99%)	3 (1%)	74	85
3	C	332/345 (96%)	321 (97%)	11 (3%)	45	56
4	D	605/643 (94%)	592 (98%)	13 (2%)	61	74
All	All	1683/1763 (96%)	1646 (98%)	37 (2%)	60	72

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	PRO
1	A	46	LEU
1	A	92	ARG
1	A	157	ASP
1	A	203	GLU
1	A	284	LEU
1	A	364	SER
1	A	400	ARG
1	A	427	ILE
1	A	536	MET
2	B	773	THR
2	B	846	GLN
2	B	926	ARG
3	C	1317	VAL
3	C	1318	CYS
3	C	1329	ASN
3	C	1405	LEU
3	C	1413	ASP
3	C	1426	VAL
3	C	1474	THR
3	C	1507	LEU
3	C	1523	LEU
3	C	1538	THR
3	C	1544	GLN

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Mol	Chain	Res	Type
4	D	48	THR
4	D	82	HIS
4	D	154	SER
4	D	167	SER
4	D	216	THR
4	D	239	ASP
4	D	293	PRO
4	D	511	SER
4	D	601	GLN
4	D	616	THR
4	D	642	ASP
4	D	654	ARG
4	D	707	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	80	GLN
3	C	1417	HIS
3	C	1430	GLN
3	C	1441	ASN
3	C	1552	ASN
4	D	82	HIS
4	D	448	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

2 carbohydrates 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	$\# Z > 2$
10	NAG	D	9097	10,4	14,14,15	0.44	0	15,19,21	1.57	1 (6%)
10	NAG	D	9098	10	14,14,15	0.46	0	15,19,21	1.36	3 (20%)

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
10	NAG	D	9097	10,4	-	0/6/23/26	0/1/1/1
10	NAG	D	9098	10	-	1/6/23/26	0/1/1/1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	D	9098	NAG	O3-C3-C2	2.02	113.12	109.11
10	D	9098	NAG	O5-C5-C6	2.28	112.29	107.35
10	D	9098	NAG	C1-O5-C5	3.41	116.57	112.25
10	D	9097	NAG	C1-O5-C5	4.64	118.14	112.25

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	D	9098	NAG	O7-C7-N2-C2

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	D	9097	NAG	1	0
10	D	9098	NAG	2	0

5.6 Ligand geometry

Of 13 ligands modelled in this entry, 3 are monoatomic - leaving 10 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	$\# Z > 2$
8	P6G	A	630	-	18,18,18	0.69	0	17,17,17	1.72	3 (17%)
5	NAG	A	9187	1	14,14,15	0.39	0	15,19,21	1.10	1 (6%)
9	PO4	B	202	-	4,4,4	0.45	0	6,6,6	0.27	0
8	P6G	C	100	-	18,18,18	0.46	0	17,17,17	1.80	4 (23%)
9	PO4	C	200	-	4,4,4	0.37	0	6,6,6	0.27	0
5	NAG	C	9324	3	14,14,15	0.60	0	15,19,21	1.31	1 (6%)
9	PO4	D	743	-	4,4,4	0.44	0	6,6,6	0.28	0
9	PO4	D	744	-	4,4,4	0.43	0	6,6,6	0.27	0
9	PO4	D	745	-	4,4,4	0.43	0	6,6,6	0.27	0
5	NAG	D	9117	4	14,14,15	0.44	0	15,19,21	1.52	2 (13%)

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
8	P6G	A	630	-	-	0/16/16/16	0/0/0/0
5	NAG	A	9187	1	-	0/6/23/26	0/1/1/1
9	PO4	B	202	-	-	0/0/0/0	0/0/0/0
8	P6G	C	100	-	-	0/16/16/16	0/0/0/0
9	PO4	C	200	-	-	0/0/0/0	0/0/0/0
5	NAG	C	9324	3	1/1/5/7	0/6/23/26	0/1/1/1
9	PO4	D	743	-	-	0/0/0/0	0/0/0/0
9	PO4	D	744	-	-	0/0/0/0	0/0/0/0
9	PO4	D	745	-	-	0/0/0/0	0/0/0/0
5	NAG	D	9117	4	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	630	P6G	O7-C6-C5	-4.70	89.47	110.36
8	C	100	P6G	C11-O10-C9	-3.92	96.46	113.31
8	C	100	P6G	O10-C11-C12	-3.82	93.40	110.36
5	D	9117	NAG	C2-N2-C7	-3.42	118.64	123.04
8	C	100	P6G	C8-O7-C6	-3.06	100.13	113.31
8	C	100	P6G	O16-C15-C14	-2.64	98.64	110.36
8	A	630	P6G	O13-C14-C15	-2.19	100.65	110.36
5	A	9187	NAG	C1-O5-C5	3.05	116.12	112.25
8	A	630	P6G	O4-C5-C6	3.06	123.95	110.36
5	D	9117	NAG	C1-O5-C5	3.37	116.52	112.25
5	C	9324	NAG	C1-O5-C5	4.10	117.45	112.25

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	C	9324	NAG	C1

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	630	P6G	3	0
5	A	9187	NAG	3	0
8	C	100	P6G	4	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	614/627 (97%)	-0.38	9 (1%) 76 75	20, 35, 63, 113	0
2	B	233/252 (92%)	-0.31	4 (1%) 73 72	22, 37, 73, 106	0
3	C	362/379 (95%)	-0.31	8 (2%) 65 64	23, 42, 80, 108	0
4	D	693/741 (93%)	-0.06	41 (5%) 26 25	22, 45, 92, 121	0
All	All	1902/1999 (95%)	-0.24	62 (3%) 50 49	20, 40, 82, 121	0

All (62) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	D	479	PRO	5.4
4	D	69	ARG	5.3
1	A	624	GLN	5.2
4	D	477	ILE	5.2
4	D	26	LEU	5.1
4	D	347	VAL	5.1
4	D	29	GLU	4.7
4	D	30	GLY	4.6
1	A	618	SER	4.3
2	B	929	ASP	4.2
4	D	612	GLU	4.1
4	D	64	ASP	3.9
4	D	478	ARG	3.9
4	D	240	PRO	3.8
4	D	27	LEU	3.7
1	A	623	PRO	3.7
4	D	25	ARG	3.7
4	D	611	GLU	3.6
3	C	1573	ASP	3.5
3	C	1382	VAL	3.4
2	B	915	VAL	3.4

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Mol	Chain	Res	Type	RSRZ
3	C	1332	LEU	3.4
4	D	708	GLN	3.4
4	D	521	ARG	3.3
4	D	67	THR	3.3
3	C	1311	LEU	3.2
4	D	707	LYS	3.2
4	D	233	LYS	3.1
4	D	447	SER	3.1
3	C	1272	TYR	3.0
3	C	1572	LYS	2.9
4	D	241	SER	2.9
2	B	934	ASP	2.9
4	D	390	ARG	2.9
4	D	520	LYS	2.9
4	D	613	LYS	2.8
4	D	671	ARG	2.7
1	A	604	LEU	2.7
1	A	249	ASP	2.7
1	A	477	ASP	2.7
4	D	352	TRP	2.7
4	D	459	HIS	2.6
3	C	1250	ASP	2.6
1	A	130	HIS	2.6
4	D	70	LYS	2.5
2	B	746	SER	2.5
4	D	740	ALA	2.5
4	D	68	VAL	2.5
4	D	490	VAL	2.4
4	D	216	THR	2.4
3	C	1333	ASN	2.4
4	D	28	GLN	2.3
1	A	74	THR	2.3
1	A	476	ARG	2.3
4	D	388	LYS	2.2
4	D	348	PRO	2.2
4	D	55	GLY	2.2
4	D	65	GLN	2.1
4	D	614	LYS	2.1
4	D	385	TYR	2.1
4	D	11	SER	2.1
4	D	90	TRP	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 ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
10	NAG	D	9097	14/15	0.89	0.21	2.47	57,74,91,94	0
10	NAG	D	9098	14/15	0.76	0.24	-	86,100,103,104	0

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	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
5	NAG	C	9324	14/15	0.71	0.21	7.57	50,76,83,85	0
8	P6G	A	630	19/19	0.75	0.27	7.17	53,85,98,98	0
5	NAG	A	9187	14/15	0.88	0.24	6.79	61,81,87,91	0
9	PO4	D	745	5/5	0.79	0.21	2.57	122,123,124,124	0
8	P6G	C	100	19/19	0.91	0.19	1.55	29,49,65,68	0
7	K	A	629	1/1	0.98	0.13	1.16	49,49,49,49	0
9	PO4	C	200	5/5	0.96	0.11	0.25	45,64,68,72	0
9	PO4	D	743	5/5	0.95	0.11	-0.01	75,79,80,80	0
6	MG	D	742	1/1	0.97	0.09	-0.86	29,29,29,29	0
6	MG	A	628	1/1	0.96	0.06	-3.06	27,27,27,27	0
9	PO4	B	202	5/5	0.92	0.12	-	106,106,108,108	0
5	NAG	D	9117	14/15	0.91	0.23	-	56,68,82,84	0
9	PO4	D	744	5/5	0.88	0.16	-	100,106,109,109	0

6.5 Other polymers [i](#)

There are no such residues in this entry.