



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 11:57 AM UTC

PDB ID : 3S9N / pdb_00003s9n
Title : Complex between transferrin receptor 1 and transferrin with iron in the N-Lobe, room temperature
Authors : Eckenroth, B.E.; Steere, A.N.; Mason, A.B.; Everse, S.J.
Deposited on : 2011-06-01
Resolution : 3.25 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

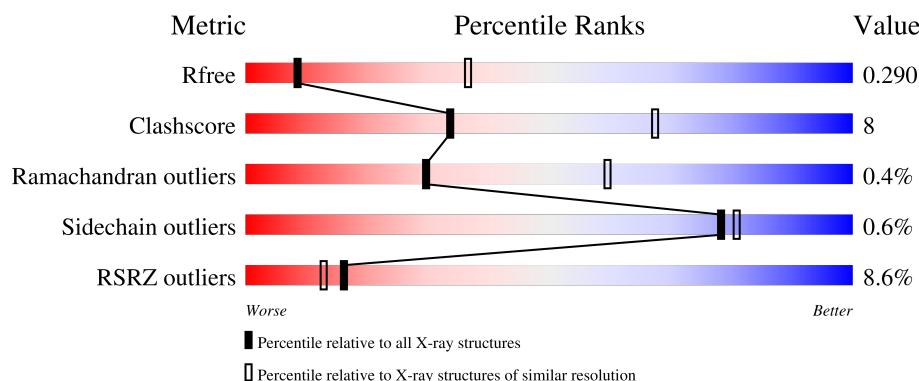
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.25 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	1605 (3.30-3.22)
Clashscore	190562	1660 (3.30-3.22)
Ramachandran outliers	187476	1630 (3.30-3.22)
Sidechain outliers	187428	1629 (3.30-3.22)
RSRZ outliers	180081	1605 (3.30-3.22)

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	654	4% 80% 16% ..
1	B	654	7% 87% 10% .
2	C	693	7% 65% 9% 26%
2	D	693	10% 61% 5% 34%

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
6	CO3	D	905	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 16304 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 Transferrin receptor protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	638	Total	C	N	O	S	0	0	0
			4917	3153	816	934	14			
1	B	639	Total	C	N	O	S	0	0	0
			4820	3092	794	922	12			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	107	VAL	-	expression tag	UNP P02786
A	108	PRO	-	expression tag	UNP P02786
A	109	ASP	-	expression tag	UNP P02786
A	110	LYS	-	expression tag	UNP P02786
A	111	HIS	-	expression tag	UNP P02786
A	112	HIS	-	expression tag	UNP P02786
A	113	HIS	-	expression tag	UNP P02786
A	114	HIS	-	expression tag	UNP P02786
A	115	HIS	-	expression tag	UNP P02786
A	116	HIS	-	expression tag	UNP P02786
A	117	ILE	-	expression tag	UNP P02786
A	118	GLU	-	expression tag	UNP P02786
A	119	GLY	-	expression tag	UNP P02786
A	142	SER	GLY	SEE REMARK 999	UNP P02786
B	107	VAL	-	expression tag	UNP P02786
B	108	PRO	-	expression tag	UNP P02786
B	109	ASP	-	expression tag	UNP P02786
B	110	LYS	-	expression tag	UNP P02786
B	111	HIS	-	expression tag	UNP P02786
B	112	HIS	-	expression tag	UNP P02786
B	113	HIS	-	expression tag	UNP P02786
B	114	HIS	-	expression tag	UNP P02786
B	115	HIS	-	expression tag	UNP P02786
B	116	HIS	-	expression tag	UNP P02786
B	117	ILE	-	expression tag	UNP P02786

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Chain	Residue	Modelled	Actual	Comment	Reference
B	118	GLU	-	expression tag	UNP P02786
B	119	GLY	-	expression tag	UNP P02786
B	142	SER	GLY	SEE REMARK 999	UNP P02786

- Molecule 2 is a protein called Serotransferrin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	511	Total	C	N	O	S	0	0	0
			3705	2328	620	721	36			
2	D	457	Total	C	N	O	S	0	0	0
			2822	1712	504	575	31			

There are 38 discrepancies between the modelled and reference sequences:

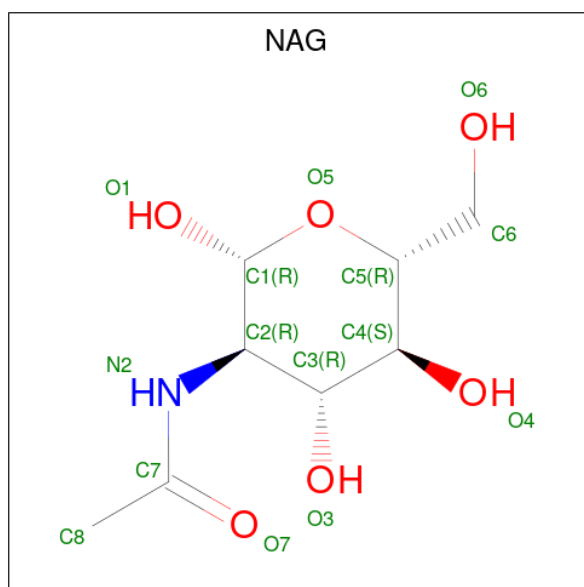
Chain	Residue	Modelled	Actual	Comment	Reference
C	-13	VAL	-	expression tag	UNP P02787
C	-12	PRO	-	expression tag	UNP P02787
C	-11	ASP	-	expression tag	UNP P02787
C	-10	LYS	-	expression tag	UNP P02787
C	-9	HIS	-	expression tag	UNP P02787
C	-8	HIS	-	expression tag	UNP P02787
C	-7	HIS	-	expression tag	UNP P02787
C	-6	HIS	-	expression tag	UNP P02787
C	-5	HIS	-	expression tag	UNP P02787
C	-4	HIS	-	expression tag	UNP P02787
C	-3	ILE	-	expression tag	UNP P02787
C	-2	GLU	-	expression tag	UNP P02787
C	-1	GLY	-	expression tag	UNP P02787
C	0	ARG	-	expression tag	UNP P02787
C	413	ASP	ASN	engineered mutation	UNP P02787
C	426	PHE	TYR	engineered mutation	UNP P02787
C	429	VAL	ILE	SEE REMARK 999	UNP P02787
C	517	PHE	TYR	engineered mutation	UNP P02787
C	611	ASP	ASN	engineered mutation	UNP P02787
D	-13	VAL	-	expression tag	UNP P02787
D	-12	PRO	-	expression tag	UNP P02787
D	-11	ASP	-	expression tag	UNP P02787
D	-10	LYS	-	expression tag	UNP P02787
D	-9	HIS	-	expression tag	UNP P02787
D	-8	HIS	-	expression tag	UNP P02787
D	-7	HIS	-	expression tag	UNP P02787
D	-6	HIS	-	expression tag	UNP P02787

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-5	HIS	-	expression tag	UNP P02787
D	-4	HIS	-	expression tag	UNP P02787
D	-3	ILE	-	expression tag	UNP P02787
D	-2	GLU	-	expression tag	UNP P02787
D	-1	GLY	-	expression tag	UNP P02787
D	0	ARG	-	expression tag	UNP P02787
D	413	ASP	ASN	engineered mutation	UNP P02787
D	426	PHE	TYR	engineered mutation	UNP P02787
D	429	VAL	ILE	SEE REMARK 999	UNP P02787
D	517	PHE	TYR	engineered mutation	UNP P02787
D	611	ASP	ASN	engineered mutation	UNP P02787

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Ca	0	0
			1	1		

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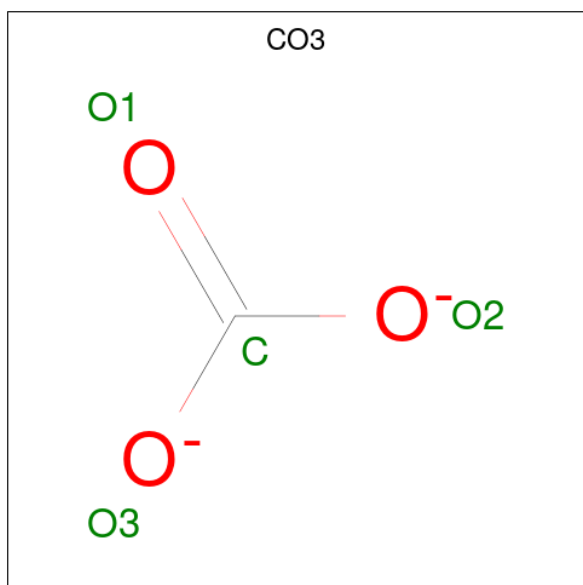
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Ca	0	0
			1	1		

- Molecule 5 is FE (III) ION (CCD ID: FE) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	1	Total	Fe	0	0
			1	1		
5	D	1	Total	Fe	0	0
			1	1		

- Molecule 6 is CARBONATE ION (CCD ID: CO3) (formula: CO₃).

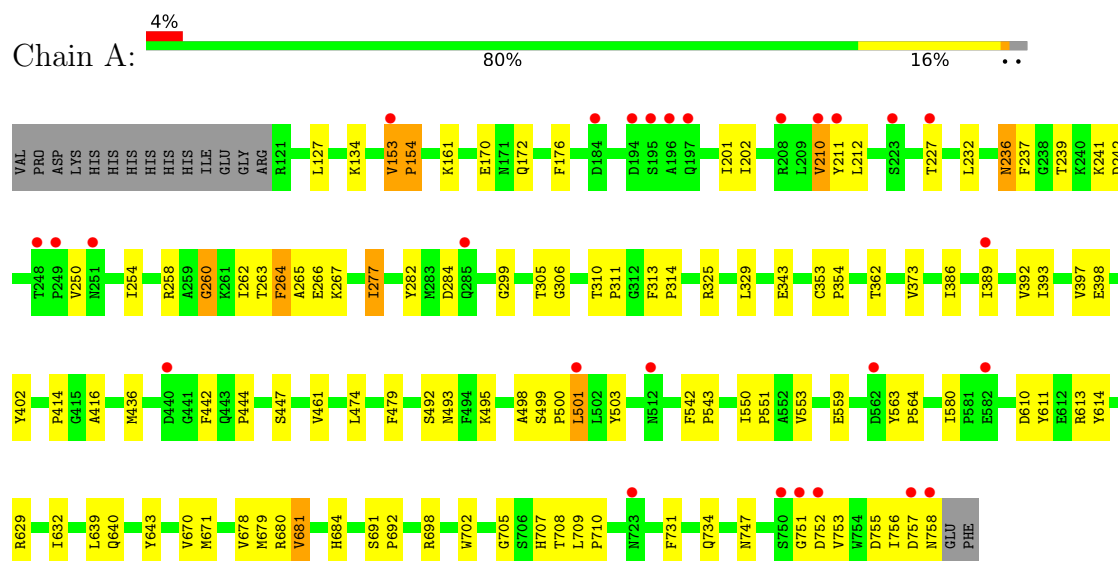


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	C	1	Total	C	O	0	0
			4	1	3		
6	D	1	Total	C	O	0	0
			4	1	3		

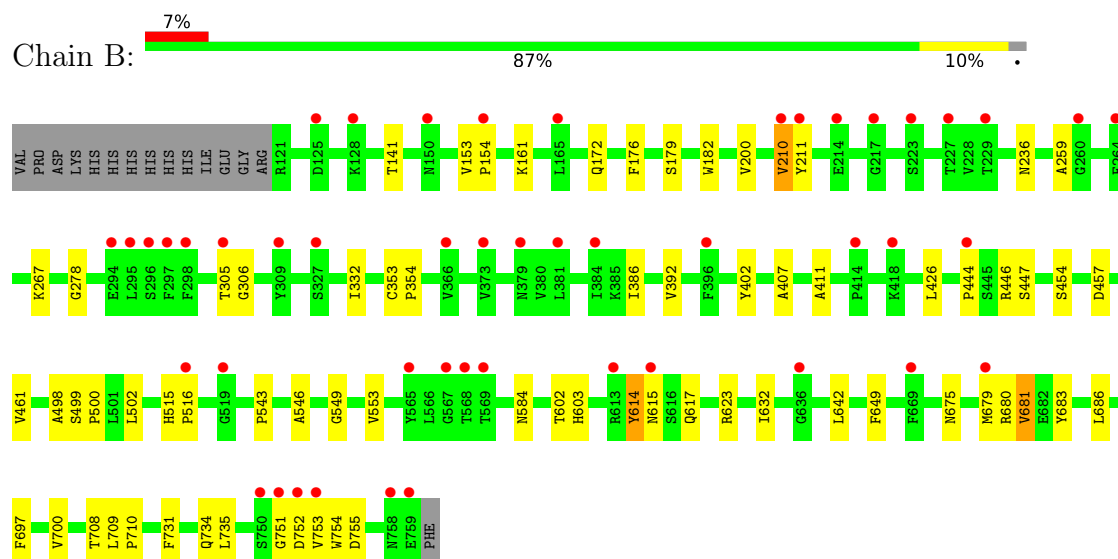
3 Residue-property plots [i](#)

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.

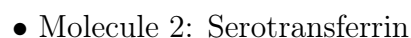
• Molecule 1: Transferrin receptor protein 1



• Molecule 1: Transferrin receptor protein 1



• Molecule 2: Serotransferrin



ARG
PRO

4 Data and refinement statistics

Property	Value	Source
Space group	P 43 2 2	Depositor
Cell constants a, b, c, α , β , γ	234.42Å 234.42Å 169.65Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 3.25 30.00 – 3.25	Depositor EDS
% Data completeness (in resolution range)	99.3 (30.00-3.25) 99.1 (30.00-3.25)	Depositor EDS
R_{merge}	0.22	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.30 (at 3.24Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.254 , 0.289 0.254 , 0.290	Depositor DCC
R_{free} test set	7501 reflections (10.13%)	wwPDB-VP
Wilson B-factor (Å ²)	91.1	Xtriage
Anisotropy	0.292	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 84.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	16304	wwPDB-VP
Average B, all atoms (Å ²)	104.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.11% 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: NAG, CA, FE, CO3

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	0.53	0/5036	0.88	8/6860 (0.1%)
1	B	0.50	0/4937	0.85	3/6744 (0.0%)
2	C	0.46	0/3784	0.80	0/5159
2	D	0.45	0/2854	0.78	0/3913
All	All	0.49	0/16611	0.84	11/22676 (0.0%)

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	752	ASP	CB-CA-C	-5.80	109.90	116.63
1	A	260	GLY	N-CA-C	5.62	117.76	112.08
1	B	236	ASN	CB-CA-C	-5.41	110.35	116.63
1	A	681	VAL	N-CA-C	5.33	116.06	110.62
1	A	580	ILE	CA-C-N	5.29	124.47	118.97
1	A	580	ILE	C-N-CA	5.29	124.47	118.97
1	A	416	ALA	N-CA-C	-5.10	107.13	113.55
1	A	236	ASN	CB-CA-C	-5.09	110.31	117.23
1	A	153	VAL	CB-CA-C	-5.04	109.01	114.35
1	B	498	ALA	N-CA-C	5.02	115.67	108.74
1	A	264	PHE	N-CA-C	-5.01	105.71	111.07

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	4917	0	4688	112	0
1	B	4820	0	4480	42	0
2	C	3705	0	3318	53	0
2	D	2822	0	2022	32	0
3	A	14	0	13	0	0
3	B	14	0	13	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
6	C	4	0	0	0	0
6	D	4	0	0	12	0
All	All	16304	0	14534	237	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 8.

All (237) 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:262:ILE:HG23	1:A:266:GLU:OE1	1.25	1.30
2:D:124:ARG:NE	6:D:905:CO3:O2	1.69	1.25
2:D:124:ARG:HG2	6:D:905:CO3:C	1.67	1.23
1:A:202:ILE:HB	1:A:210:VAL:HG11	1.30	1.10
1:A:134:LYS:HE3	1:A:436:MET:HG3	1.39	1.02
2:C:130:ILE:HD11	2:C:246:VAL:CG2	1.88	1.01
2:D:124:ARG:CG	6:D:905:CO3:O2	2.10	1.00
1:A:262:ILE:CG2	1:A:266:GLU:OE1	2.11	0.97
1:A:442:PHE:CE2	1:A:444:PRO:HG3	2.00	0.96
2:D:124:ARG:CG	6:D:905:CO3:C	2.48	0.91
2:D:124:ARG:CD	6:D:905:CO3:O2	2.19	0.90
2:D:124:ARG:HG2	6:D:905:CO3:O2	1.67	0.88
1:A:262:ILE:HG22	1:A:263:THR:N	1.88	0.87
1:A:492:SER:OG	1:A:559:GLU:OE2	1.95	0.84
2:C:49:ILE:HD11	2:C:62:LEU:HD21	1.59	0.83
1:B:751:GLY:O	1:B:755:ASP:HB2	1.78	0.83
1:A:263:THR:HG22	1:A:265:ALA:H	1.44	0.82
1:A:325:ARG:CG	1:A:329:LEU:HD12	2.09	0.81
2:C:246:VAL:HG13	2:C:247:PRO:HD2	1.61	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:753:VAL:HG12	1:A:753:VAL:O	1.81	0.81
1:B:386:ILE:HG23	1:B:454:SER:HB3	1.63	0.80
1:A:202:ILE:HB	1:A:210:VAL:CG1	2.12	0.78
2:C:130:ILE:HD11	2:C:246:VAL:HG23	1.65	0.77
1:A:262:ILE:CG2	1:A:263:THR:N	2.47	0.77
1:A:134:LYS:HE3	1:A:436:MET:CG	2.15	0.76
1:A:202:ILE:CB	1:A:210:VAL:HG11	2.11	0.76
1:A:751:GLY:O	1:A:755:ASP:HB2	1.85	0.76
1:A:262:ILE:CG2	1:A:263:THR:H	1.99	0.74
1:A:263:THR:HG22	1:A:265:ALA:N	2.02	0.74
1:A:325:ARG:HG3	1:A:329:LEU:CD1	2.18	0.74
1:A:210:VAL:HG12	1:A:211:TYR:H	1.52	0.73
1:A:202:ILE:HG22	1:A:210:VAL:HG21	1.70	0.73
2:D:124:ARG:HG2	6:D:905:CO3:O3	1.88	0.73
1:B:154:PRO:HD2	1:B:161:LYS:HG3	1.70	0.73
2:D:338:GLU:O	2:D:339:CYS:HB2	1.89	0.72
1:A:202:ILE:O	1:A:210:VAL:HB	1.89	0.72
2:C:130:ILE:N	2:C:131:PRO:HD2	2.05	0.72
1:B:753:VAL:HG22	1:B:753:VAL:O	1.89	0.71
2:C:105:SER:HB2	2:C:232:ARG:HH22	1.56	0.69
1:A:325:ARG:HG2	1:A:329:LEU:HD12	1.71	0.69
1:A:325:ARG:CG	1:A:329:LEU:CD1	2.70	0.68
2:C:12:SER:HB2	2:C:180:SER:HB2	1.76	0.68
2:D:406:PRO:O	2:D:641:LEU:CD1	2.41	0.68
1:B:153:VAL:HB	1:B:154:PRO:HD3	1.76	0.68
2:D:406:PRO:O	2:D:641:LEU:HD11	1.94	0.67
1:A:262:ILE:HG22	1:A:266:GLU:HB2	1.76	0.66
1:A:262:ILE:CG2	1:A:266:GLU:HB2	2.25	0.66
1:A:262:ILE:HG22	1:A:263:THR:H	1.58	0.66
2:C:130:ILE:HD11	2:C:246:VAL:HG21	1.76	0.66
1:B:615:ASN:OD1	1:B:649:PHE:HD2	1.80	0.65
1:B:182:TRP:HZ3	1:B:392:VAL:HG12	1.60	0.65
2:D:124:ARG:CD	6:D:905:CO3:C	2.73	0.64
1:A:210:VAL:HG12	1:A:211:TYR:N	2.11	0.64
1:A:757:ASP:O	1:A:758:ASN:C	2.39	0.64
1:A:479:PHE:HB3	1:A:679:MET:HE3	1.78	0.64
1:A:753:VAL:O	1:A:753:VAL:CG1	2.46	0.64
2:C:612:VAL:HG12	2:C:613:THR:H	1.63	0.63
1:A:239:THR:HB	1:A:242:ASP:OD1	1.99	0.63
1:A:258:ARG:HD2	1:A:284:ASP:OD2	1.98	0.63
2:C:206:LYS:NZ	2:C:298:SER:OG	2.31	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:663:ARG:CB	2:D:671:LEU:HD21	2.29	0.62
2:C:125:SER:CB	2:C:246:VAL:HG11	2.30	0.62
1:A:614:TYR:HH	1:A:702:TRP:HZ3	1.43	0.62
1:A:134:LYS:CE	1:A:436:MET:HG3	2.22	0.61
2:C:130:ILE:H	2:C:131:PRO:HD2	1.66	0.61
1:A:501:LEU:HD23	1:A:611:TYR:HA	1.82	0.61
1:A:153:VAL:CB	1:A:154:PRO:HD3	2.31	0.59
1:A:500:PRO:O	1:A:503:TYR:HB2	2.01	0.59
2:C:246:VAL:CG1	2:C:247:PRO:HD2	2.31	0.59
1:B:179:SER:HB2	1:B:392:VAL:O	2.02	0.59
2:C:5:THR:HG22	2:C:36:SER:HB3	1.85	0.59
2:D:598:HIS:HE1	2:D:640:LYS:CB	2.15	0.59
2:C:246:VAL:HG13	2:C:247:PRO:CD	2.32	0.59
2:D:643:ASP:HB2	2:D:645:ASN:OD1	2.03	0.58
1:A:250:VAL:HG12	1:A:250:VAL:O	2.04	0.57
2:D:124:ARG:CG	6:D:905:CO3:O3	2.47	0.57
2:D:358:TRP:CZ2	2:D:366:ILE:HD13	2.39	0.57
1:A:262:ILE:CG2	1:A:266:GLU:CB	2.82	0.57
2:C:130:ILE:N	2:C:131:PRO:CD	2.66	0.57
1:B:614:TYR:O	1:B:617:GLN:HB2	2.05	0.56
1:B:708:THR:HB	1:B:710:PRO:HD2	1.88	0.56
2:C:105:SER:H	2:C:232:ARG:HH12	1.54	0.56
2:C:125:SER:HB3	2:C:246:VAL:HG11	1.87	0.56
2:D:351:GLU:HG3	2:D:629:LEU:O	2.04	0.56
1:A:210:VAL:CG1	1:A:211:TYR:H	2.13	0.56
1:A:263:THR:O	1:A:267:LYS:HG3	2.06	0.56
1:A:708:THR:HB	1:A:710:PRO:HD2	1.87	0.56
1:A:262:ILE:HG23	1:A:266:GLU:CD	2.20	0.56
1:B:680:ARG:O	1:B:683:TYR:N	2.39	0.55
1:B:642:LEU:HD11	1:B:735:LEU:HD11	1.89	0.55
1:B:306:GLY:HA2	1:B:461:VAL:HA	1.88	0.54
2:C:109:MET:HE3	2:C:243:LEU:HD21	1.90	0.54
2:C:130:ILE:CD1	2:C:246:VAL:CG2	2.76	0.54
1:A:153:VAL:CB	1:A:154:PRO:CD	2.85	0.54
2:C:136:TYR:OH	2:C:329:GLY:HA2	2.07	0.54
2:D:124:ARG:NE	6:D:905:CO3:C	2.65	0.54
1:A:227:THR:O	1:A:227:THR:HG23	2.07	0.54
1:A:402:TYR:HB3	1:A:447:SER:HB2	1.90	0.53
1:A:201:ILE:HG22	1:A:212:LEU:HA	1.90	0.53
2:D:626:THR:OG1	2:D:629:LEU:HD21	2.09	0.53
2:C:400:GLY:HA3	2:C:647:TYR:HB3	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:124:ARG:CD	6:D:905:CO3:O3	2.57	0.53
1:A:747:ASN:HB3	1:A:756:ILE:HD13	1.89	0.53
1:B:141:THR:HG22	1:B:584:ASN:HD22	1.74	0.52
2:C:246:VAL:CG1	2:C:247:PRO:CD	2.87	0.52
2:C:128:TRP:C	2:C:131:PRO:HD2	2.34	0.52
1:A:306:GLY:HA2	1:A:461:VAL:HA	1.92	0.51
1:A:210:VAL:HG12	1:A:211:TYR:CD2	2.46	0.51
2:C:377:CYS:HB3	2:C:389:MET:SD	2.51	0.51
1:B:680:ARG:O	1:B:681:VAL:C	2.54	0.51
1:A:501:LEU:CD2	1:A:611:TYR:HA	2.40	0.50
1:B:753:VAL:HG13	1:B:754:TRP:CE3	2.46	0.50
1:A:731:PHE:HA	1:A:734:GLN:HE21	1.76	0.50
1:B:731:PHE:HA	1:B:734:GLN:HE21	1.75	0.50
1:A:680:ARG:HB3	1:A:684:HIS:CE1	2.47	0.50
1:A:262:ILE:HG21	1:A:266:GLU:CB	2.41	0.50
1:B:515:HIS:CG	1:B:516:PRO:HD2	2.48	0.49
1:A:254:ILE:HD12	1:A:373:VAL:HG23	1.93	0.49
2:C:179:CYS:O	2:C:186:PHE:CE1	2.66	0.49
1:A:262:ILE:CG2	1:A:266:GLU:CD	2.83	0.49
2:C:37:VAL:HG22	2:C:266:LEU:HD21	1.94	0.49
1:A:172:GLN:HG3	1:A:176:PHE:CZ	2.47	0.49
1:B:402:TYR:HB3	1:B:447:SER:HB2	1.94	0.49
1:B:305:THR:HG21	1:B:543:PRO:HG3	1.93	0.49
1:A:501:LEU:HD23	1:A:610:ASP:C	2.38	0.48
2:C:293:LEU:O	2:C:295:PHE:N	2.46	0.48
1:A:501:LEU:HD23	1:A:610:ASP:O	2.13	0.47
1:A:343:GLU:HG2	1:A:362:THR:HG21	1.95	0.47
2:C:52:ILE:HG22	2:C:254:ARG:HG3	1.96	0.47
1:B:753:VAL:O	1:B:753:VAL:CG2	2.59	0.47
1:A:542:PHE:HB3	1:A:543:PRO:HD3	1.97	0.47
1:A:258:ARG:HH11	1:A:284:ASP:CG	2.22	0.47
1:A:493:ASN:HD21	1:A:495:LYS:HE2	1.79	0.47
1:A:153:VAL:O	1:A:414:PRO:HA	2.14	0.47
1:A:232:LEU:HA	1:A:254:ILE:O	2.14	0.47
2:C:52:ILE:HD11	2:C:60:VAL:HG12	1.97	0.47
1:A:262:ILE:HG21	1:A:266:GLU:HB3	1.97	0.47
1:A:500:PRO:HG2	1:A:614:TYR:CZ	2.50	0.47
1:B:623:ARG:HD3	2:D:363:VAL:HG22	1.96	0.47
1:B:700:VAL:HB	1:B:709:LEU:HD13	1.97	0.47
2:D:124:ARG:HD3	6:D:905:CO3:O3	2.14	0.47
1:A:474:LEU:HD13	1:A:550:ILE:HD11	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:406:PRO:HA	2:C:588:VAL:HA	1.96	0.46
1:A:500:PRO:CD	1:A:702:TRP:CH2	2.98	0.46
2:C:125:SER:OG	2:C:246:VAL:HG11	2.14	0.46
2:C:130:ILE:H	2:C:131:PRO:CD	2.28	0.46
1:A:262:ILE:HG23	1:A:263:THR:H	1.80	0.46
1:A:305:THR:HG21	1:A:543:PRO:HG3	1.98	0.46
1:B:502:LEU:HD13	1:B:553:VAL:HB	1.98	0.46
2:C:206:LYS:HG2	2:C:207:HIS:H	1.81	0.46
1:B:259:ALA:HA	1:B:267:LYS:HE3	1.97	0.46
2:C:408:LEU:HB2	2:C:587:VAL:HB	1.97	0.46
1:A:498:ALA:HB2	1:A:553:VAL:HG23	1.97	0.46
1:A:250:VAL:O	1:A:250:VAL:CG1	2.64	0.45
2:C:135:LEU:O	2:C:139:LEU:HG	2.16	0.45
1:A:670:VAL:HG13	1:A:671:MET:N	2.31	0.45
1:A:640:GLN:HA	1:A:643:TYR:HD1	1.81	0.45
1:B:411:ALA:HA	1:B:457:ASP:OD2	2.16	0.45
2:C:225:LEU:HD13	2:C:235:VAL:HA	1.98	0.45
2:C:59:ALA:HB2	2:C:263:ILE:HD13	1.99	0.45
2:C:646:THR:H	2:C:649:LYS:HB2	1.81	0.45
1:A:154:PRO:O	1:A:161:LYS:CB	2.64	0.45
2:C:246:VAL:HG12	2:C:247:PRO:N	2.31	0.45
2:C:624:SER:HB3	2:C:629:LEU:HD13	1.97	0.45
1:A:239:THR:HG22	1:A:241:LYS:H	1.81	0.45
1:B:499:SER:O	1:B:500:PRO:C	2.59	0.45
2:D:641:LEU:O	2:D:642:HIS:CB	2.63	0.45
2:D:306:PRO:HA	2:D:307:PRO:HD3	1.79	0.44
1:A:258:ARG:HG2	1:A:282:TYR:CZ	2.52	0.44
1:A:705:GLY:HA3	1:A:707:HIS:CE1	2.52	0.44
1:A:258:ARG:HD2	1:A:284:ASP:CG	2.42	0.44
2:D:406:PRO:O	2:D:641:LEU:HD12	2.16	0.44
1:A:362:THR:O	1:A:362:THR:HG22	2.17	0.44
1:A:392:VAL:HG22	1:A:393:ILE:N	2.31	0.44
2:D:130:ILE:N	2:D:131:PRO:HD2	2.31	0.44
1:A:310:THR:N	1:A:311:PRO:HD3	2.32	0.44
2:C:347:LEU:HD22	2:C:374:THR:HA	1.99	0.44
1:A:691:SER:HA	1:A:692:PRO:HD3	1.85	0.44
2:C:391:LEU:HD12	2:C:588:VAL:HG21	2.00	0.44
1:A:692:PRO:HG3	1:A:698:ARG:HD3	2.00	0.44
2:D:174:CYS:HA	2:D:175:PRO:HD3	1.86	0.44
1:A:500:PRO:HD3	1:A:702:TRP:CH2	2.53	0.44
1:B:172:GLN:HG3	1:B:176:PHE:CE2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:444:PRO:HB3	1:B:602:THR:HG21	2.00	0.43
2:C:612:VAL:C	2:C:614:ASP:H	2.26	0.43
2:D:69:ASP:HA	2:D:72:LEU:HD12	2.00	0.43
1:A:503:TYR:HB2	1:A:613:ARG:HD2	2.00	0.43
1:A:397:VAL:HG12	1:A:398:GLU:HG3	2.01	0.43
1:B:278:GLY:HA2	1:B:332:ILE:HG23	2.01	0.43
1:B:753:VAL:HG13	1:B:754:TRP:HE3	1.83	0.43
1:B:753:VAL:CG1	1:B:754:TRP:CE3	3.02	0.43
1:A:260:GLY:C	1:A:262:ILE:H	2.22	0.43
1:B:172:GLN:HG3	1:B:176:PHE:CZ	2.54	0.43
2:C:130:ILE:CD1	2:C:246:VAL:HG21	2.46	0.43
1:A:709:LEU:N	1:A:710:PRO:CD	2.82	0.42
1:B:751:GLY:C	1:B:755:ASP:HB2	2.43	0.42
1:A:499:SER:OG	1:A:500:PRO:HD2	2.18	0.42
2:C:130:ILE:CD1	2:C:246:VAL:HG23	2.41	0.42
1:A:277:ILE:H	1:A:277:ILE:HG13	1.67	0.42
1:A:678:VAL:O	1:A:681:VAL:HG22	2.20	0.42
1:B:200:VAL:O	1:B:200:VAL:HG13	2.20	0.42
1:A:752:ASP:HB3	1:A:753:VAL:H	1.61	0.42
1:A:134:LYS:CE	1:A:436:MET:CG	2.90	0.41
1:A:170:GLU:HB2	1:A:389:ILE:HD13	2.02	0.41
2:D:176:GLY:O	2:D:177:CYS:HB2	2.19	0.41
2:D:400:GLY:HA3	2:D:647:TYR:HB3	2.01	0.41
1:A:264:PHE:CE1	1:A:299:GLY:HA3	2.55	0.41
2:C:246:VAL:CG1	2:C:247:PRO:N	2.83	0.41
1:B:353:CYS:HA	1:B:354:PRO:HD3	1.84	0.41
1:B:446:ARG:H	1:B:602:THR:HG23	1.85	0.41
1:B:549:GLY:HA3	1:B:686:LEU:HD11	2.02	0.41
1:A:263:THR:CG2	1:A:264:PHE:N	2.84	0.41
1:B:546:ALA:HB1	1:B:697:PHE:HB3	2.02	0.41
2:D:63:ASP:HA	2:D:249:HIS:ND1	2.35	0.41
1:A:632:ILE:HD13	1:A:639:LEU:HD13	2.02	0.41
1:B:675:ASN:O	1:B:679:MET:HG3	2.21	0.41
2:C:48:CYS:HB3	2:C:60:VAL:HG11	2.03	0.41
1:A:614:TYR:OH	1:A:702:TRP:CZ3	2.68	0.41
1:A:263:THR:HG22	1:A:264:PHE:N	2.35	0.41
1:A:313:PHE:HB2	1:A:314:PRO:HD2	2.02	0.41
1:A:670:VAL:CG1	1:A:671:MET:N	2.83	0.41
1:B:210:VAL:HG12	1:B:211:TYR:N	2.35	0.41
1:B:407:ALA:HB3	1:B:426:LEU:HD22	2.03	0.41
1:A:236:ASN:CG	1:A:237:PHE:H	2.29	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:479:PHE:O	1:A:551:PRO:HD2	2.21	0.40
1:A:629:ARG:NH2	2:C:618:ASN:OD1	2.52	0.40
1:A:563:TYR:HA	1:A:564:PRO:HD3	1.83	0.40
2:C:206:LYS:HG2	2:C:207:HIS:N	2.35	0.40
2:D:624:SER:HB3	2:D:626:THR:O	2.21	0.40
1:A:353:CYS:HA	1:A:354:PRO:HD3	1.84	0.40
1:A:442:PHE:CZ	1:A:444:PRO:HG3	2.51	0.40
2:C:319:TYR:O	2:C:323:ILE:HG13	2.21	0.40
2:C:345:CYS:HA	2:C:369:VAL:O	2.21	0.40
1:A:202:ILE:CG2	1:A:210:VAL:HG11	2.49	0.40
1:A:264:PHE:O	1:A:267:LYS:HB2	2.20	0.40
1:A:614:TYR:OH	1:A:702:TRP:HZ3	2.02	0.40
2:C:306:PRO:HA	2:C:307:PRO:HD3	1.81	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	636/654 (97%)	604 (95%)	30 (5%)	2 (0%)	36	66
1	B	637/654 (97%)	607 (95%)	28 (4%)	2 (0%)	36	66
2	C	505/693 (73%)	474 (94%)	29 (6%)	2 (0%)	30	59
2	D	431/693 (62%)	400 (93%)	29 (7%)	2 (0%)	24	55
All	All	2209/2694 (82%)	2085 (94%)	116 (5%)	8 (0%)	30	59

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	681	VAL
2	D	628	ASP

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Mol	Chain	Res	Type
1	A	154	PRO
1	A	210	VAL
1	B	210	VAL
2	C	628	ASP
2	C	613	THR
2	D	339	CYS

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	512/562 (91%)	508 (99%)	4 (1%)	73	78
1	B	483/562 (86%)	480 (99%)	3 (1%)	78	81
2	C	366/585 (63%)	364 (100%)	2 (0%)	81	82
2	D	189/585 (32%)	189 (100%)	0	100	100
All	All	1550/2294 (68%)	1541 (99%)	9 (1%)	78	81

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	127	LEU
1	A	277	ILE
1	A	386	ILE
1	A	501	LEU
1	B	603	HIS
1	B	614	TYR
1	B	632	ILE
2	C	377	CYS
2	C	612	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (45) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	148	ASN

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Mol	Chain	Res	Type
1	A	160	GLN
1	A	164	ASN
1	A	318	HIS
1	A	320	GLN
1	A	401	HIS
1	A	431	GLN
1	A	475	HIS
1	A	483	ASN
1	A	511	GLN
1	A	512	ASN
1	A	596	GLN
1	A	626	ASN
1	A	684	HIS
1	A	721	GLN
1	A	734	GLN
1	A	743	GLN
1	A	747	ASN
1	A	758	ASN
1	B	148	ASN
1	B	164	ASN
1	B	401	HIS
1	B	431	GLN
1	B	483	ASN
1	B	524	GLN
1	B	584	ASN
1	B	596	GLN
1	B	603	HIS
1	B	626	ASN
1	B	727	ASN
1	B	734	GLN
1	B	743	GLN
1	B	747	ASN
2	C	207	HIS
2	C	230	ASN
2	C	269	GLN
2	C	300	HIS
2	C	349	HIS
2	C	361	ASN
2	C	584	ASN
2	C	604	GLN
2	D	584	ASN
2	D	598	HIS

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Mol	Chain	Res	Type
2	D	604	GLN
2	D	605	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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	NAG	B	903	1	14,14,15	0.44	0	17,19,21	1.17	2 (11%)
3	NAG	A	903	1	14,14,15	0.43	0	17,19,21	1.15	2 (11%)
6	CO3	C	905	5	3,3,3	0.33	0	2,3,3	0.48	0
6	CO3	D	905	5	3,3,3	0.28	0	2,3,3	0.21	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	B	903	1	-	0/6/23/26	0/1/1/1
3	NAG	A	903	1	-	0/6/23/26	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($^{\circ}$)	Ideal($^{\circ}$)
3	B	903	NAG	C8-C7-N2	2.33	119.98	116.12
3	A	903	NAG	C8-C7-N2	2.30	119.93	116.12
3	B	903	NAG	C2-N2-C7	-2.21	119.94	122.90
3	A	903	NAG	C2-N2-C7	-2.18	119.97	122.90

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	D	905	CO3	12	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	638/654 (97%)	0.31	27 (4%)	40	26	39, 75, 125, 200	0
1	B	639/654 (97%)	0.59	48 (7%)	20	15	38, 92, 162, 200	1 (0%)
2	C	511/693 (73%)	0.78	50 (9%)	13	10	65, 112, 172, 200	0
2	D	457/693 (65%)	0.98	68 (14%)	5	5	67, 153, 192, 200	0
All	All	2245/2694 (83%)	0.63	193 (8%)	16	13	38, 100, 179, 200	1 (0%)

All (193) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	752	ASP	5.3
1	B	217	GLY	5.1
2	D	131	PRO	5.0
2	D	267	LEU	4.9
2	D	583	PRO	4.9
1	B	751	GLY	4.9
1	A	208	ARG	4.6
1	B	154	PRO	4.4
1	A	750	SER	4.0
1	A	196	ALA	4.0
2	D	96	TYR	3.9
1	A	197	GLN	3.9
2	C	107	PHE	3.9
1	A	153	VAL	3.9
2	D	207	HIS	3.8
1	B	366	VAL	3.8
1	B	229	THR	3.8
1	A	751	GLY	3.8
1	B	396	PHE	3.8
2	D	39	CYS	3.8
2	D	258	GLY	3.7

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Mol	Chain	Res	Type	RSRZ
2	D	127	GLY	3.7
1	B	295	LEU	3.6
1	B	636	GLY	3.6
1	A	211	TYR	3.6
1	B	128	LYS	3.6
2	D	393	GLY	3.6
2	D	636	VAL	3.6
1	B	373	VAL	3.6
2	C	99	ALA	3.5
2	D	641	LEU	3.5
2	C	97	ALA	3.4
2	C	677	ARG	3.4
2	C	28	SER	3.3
1	A	512	ASN	3.3
2	C	189	SER	3.3
2	C	658	ALA	3.3
1	A	195	SER	3.2
1	B	294	GLU	3.2
1	B	613	ARG	3.1
1	B	753	VAL	3.1
2	D	313	MET	3.1
2	C	329	GLY	3.1
2	D	61	THR	3.1
2	D	292	ASP	3.1
2	C	640	LYS	3.1
1	A	227	THR	3.0
1	B	264	PHE	3.0
1	B	565	TYR	3.0
2	D	388	ALA	3.0
2	D	297	ASP	3.0
2	C	59	ALA	2.9
2	D	244	ALA	2.9
2	C	610	SER	2.9
1	B	567	GLY	2.9
1	B	223	SER	2.9
2	C	237	GLU	2.9
1	B	752	ASP	2.9
1	A	758	ASN	2.9
2	C	383	ASN	2.9
1	A	223	SER	2.8
1	A	194	ASP	2.8
2	D	65	GLY	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	296	SER	2.8
1	B	444	PRO	2.8
1	A	501	LEU	2.8
2	D	394	GLY	2.8
1	A	251	ASN	2.7
2	C	136	TYR	2.7
2	C	665	CYS	2.7
1	A	248	THR	2.7
1	B	750	SER	2.7
2	C	141	GLU	2.7
1	B	298	PHE	2.7
2	D	345	CYS	2.6
2	C	246	VAL	2.6
2	D	630	LEU	2.6
2	C	53	ALA	2.6
2	D	11	VAL	2.6
2	D	98	VAL	2.6
2	D	190	GLY	2.6
2	D	648	GLU	2.6
2	C	185	TYR	2.6
2	C	238	TYR	2.6
1	B	214	GLU	2.6
2	C	583	PRO	2.5
2	D	370	SER	2.5
2	C	172	GLN	2.5
1	B	305	THR	2.5
2	C	330	THR	2.5
2	D	68	TYR	2.5
2	D	158	CYS	2.5
2	D	294	LEU	2.5
2	D	128	TRP	2.5
1	B	759	GLU	2.5
2	D	411	ASN	2.5
1	B	679	MET	2.5
1	B	260	GLY	2.5
1	B	615	ASN	2.5
2	D	223	TYR	2.5
2	C	156	GLY	2.5
2	D	616	SER	2.4
2	C	225	LEU	2.4
1	B	309	TYR	2.4
2	C	647	TYR	2.4

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Mol	Chain	Res	Type	RSRZ
2	C	224	GLU	2.4
2	D	314	TYR	2.4
2	C	211	PHE	2.4
2	D	300	HIS	2.4
2	C	228	LEU	2.4
2	C	291	LYS	2.4
2	D	423	GLU	2.4
1	B	210	VAL	2.4
2	D	652	GLY	2.3
1	A	389	ILE	2.3
1	A	184	ASP	2.3
1	B	516	PRO	2.3
2	C	210	ILE	2.3
2	D	642	HIS	2.3
1	B	211	TYR	2.3
2	D	318	GLU	2.3
2	D	206	LYS	2.3
2	C	168	PRO	2.3
1	B	165	LEU	2.3
2	D	6	VAL	2.3
1	A	210	VAL	2.3
2	D	405	VAL	2.3
2	C	86	GLY	2.3
2	D	389	MET	2.3
2	D	266	LEU	2.3
2	D	298	SER	2.3
1	A	723	ASN	2.3
1	B	758	ASN	2.3
1	A	440	ASP	2.3
1	B	125	ASP	2.3
2	D	79	PRO	2.2
1	A	562	ASP	2.2
2	C	351	GLU	2.2
2	D	156	GLY	2.2
2	D	232	ARG	2.2
2	C	612	VAL	2.2
2	D	173	LEU	2.2
1	B	418	LYS	2.2
2	C	622	PHE	2.2
2	D	667	THR	2.2
2	D	397	TYR	2.2
2	D	205	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	327	SER	2.2
2	D	28	SER	2.2
2	D	422	PRO	2.2
2	C	5	THR	2.2
2	C	653	GLU	2.2
2	C	644	ARG	2.2
2	C	598	HIS	2.2
2	D	242	HIS	2.2
1	B	568	THR	2.1
2	D	639	ALA	2.1
1	A	249	PRO	2.1
2	C	74	PRO	2.1
2	D	86	GLY	2.1
2	D	168	PRO	2.1
2	D	295	PHE	2.1
1	A	757	ASP	2.1
2	C	161	CYS	2.1
2	D	339	CYS	2.1
1	B	227	THR	2.1
1	B	669	PHE	2.1
2	D	208	SER	2.1
2	C	213	ASN	2.1
1	B	381	LEU	2.1
1	B	384	ILE	2.1
2	C	347	LEU	2.1
2	D	418	CYS	2.1
1	B	569	THR	2.1
2	D	64	ALA	2.1
1	A	582	GLU	2.1
2	D	396	VAL	2.1
1	B	379	ASN	2.1
2	C	4	LYS	2.1
2	D	8	TRP	2.1
2	C	85	TYR	2.1
2	C	659	VAL	2.0
1	B	297	PHE	2.0
1	B	519	GLY	2.0
2	D	605	GLN	2.0
2	C	135	LEU	2.0
2	C	173	LEU	2.0
1	B	150	ASN	2.0
2	D	647	TYR	2.0

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Mol	Chain	Res	Type	RSRZ
2	D	622	PHE	2.0
1	A	285	GLN	2.0
1	B	414	PRO	2.0
2	C	654	GLU	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	NAG	B	903	14/15	0.54	0.26	126,126,126,126	0
3	NAG	A	903	14/15	0.66	0.26	124,124,124,124	0
6	CO3	D	905	4/4	0.83	0.10	96,96,96,96	0
6	CO3	C	905	4/4	0.85	0.15	96,96,96,96	0
4	CA	A	900	1/1	0.94	0.09	96,96,96,96	0
4	CA	B	900	1/1	0.94	0.07	96,96,96,96	0
5	FE	C	901	1/1	0.96	0.06	96,96,96,96	0
5	FE	D	901	1/1	0.96	0.09	96,96,96,96	0

6.5 Other polymers [i](#)

There are no such residues in this entry.