Full wwPDB X-ray Structure Validation Report ⓘ

Jun 16, 2024 – 11:20 PM EDT

PDB ID	:	3S9N
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:

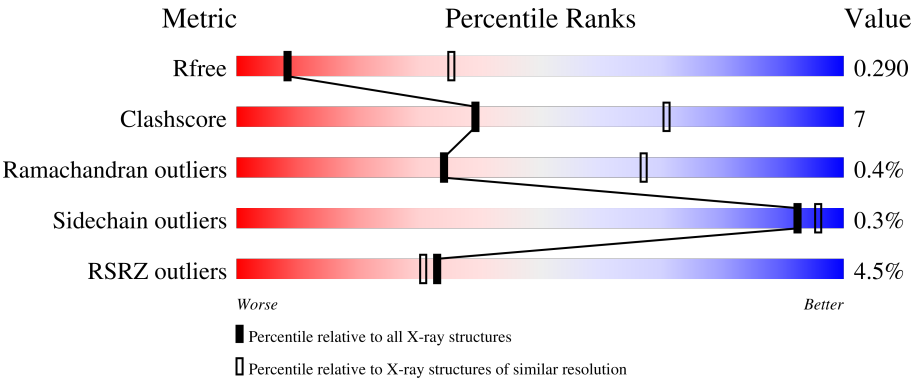
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

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}	130704	1191 (3.30-3.22)
Clashscore	141614	1251 (3.30-3.22)
Ramachandran outliers	138981	1229 (3.30-3.22)
Sidechain outliers	138945	1228 (3.30-3.22)
RSRZ outliers	127900	1154 (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 <=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	2% 81% 16% ·
1	B	654	2% 88% 9% ·
2	C	693	2% 65% 9% 26%
2	D	693	8% 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 (i)

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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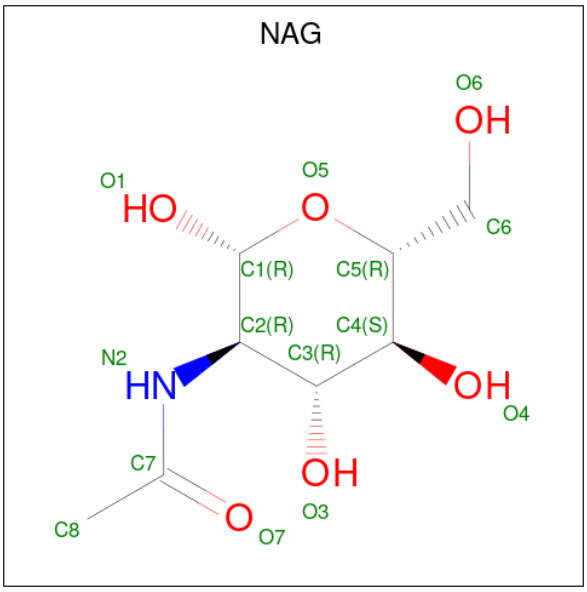
Chain	Residue	Modelled	Actual	Comment	Reference
D	-5	HIS	-	expression tag	UNP P02787
D	-4	HIS	-	expression tag	UNP P02787
D	-3	ILE	-	expression tag	UNP P02787
D	-2	GLU	-	expression tag	UNP P02787
D	-1	GLY	-	expression tag	UNP P02787
D	0	ARG	-	expression tag	UNP P02787
D	413	ASP	ASN	engineered mutation	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 (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

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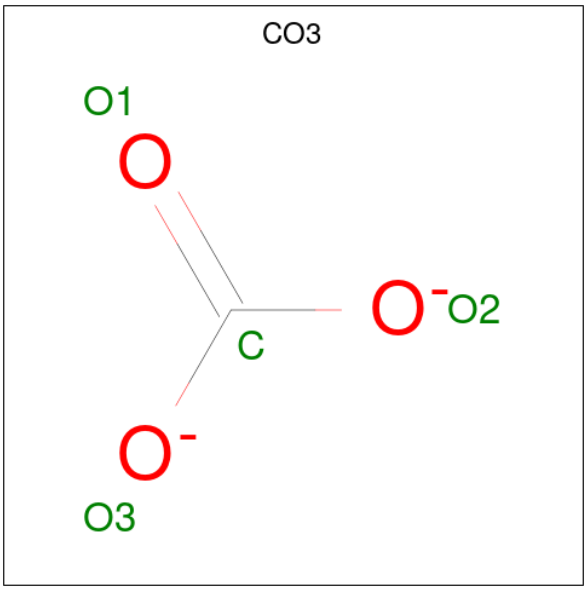
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total Ca 1 1	0	0

- Molecule 5 is FE (III) ION (three-letter code: FE) (formula: Fe).

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

- Molecule 6 is CARBONATE ION (three-letter code: CO3) (formula: CO_3).



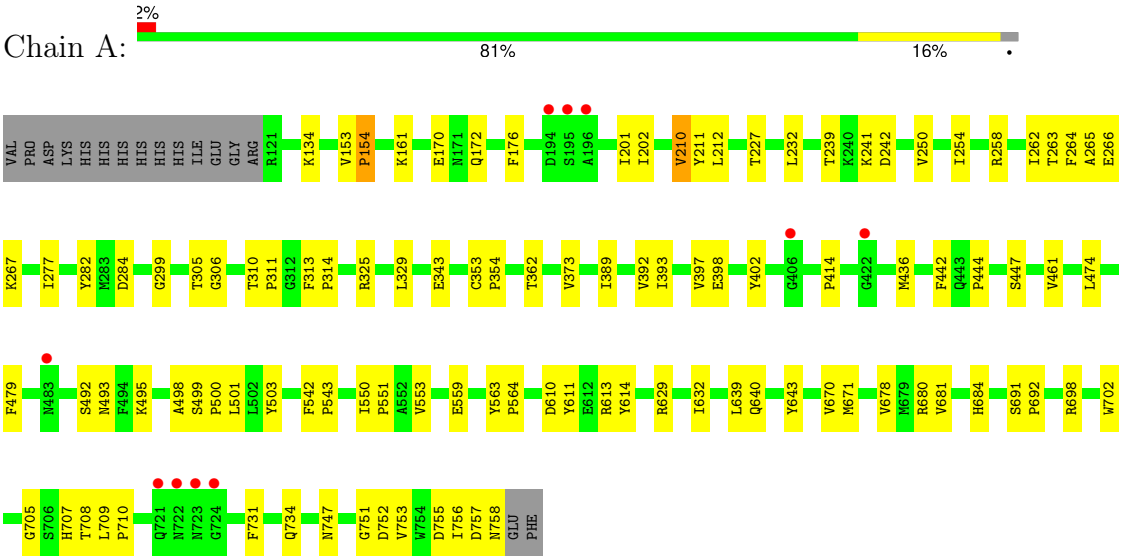
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	C	1	Total C O 4 1 3	0	0
6	D	1	Total C O 4 1 3	0	0

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.

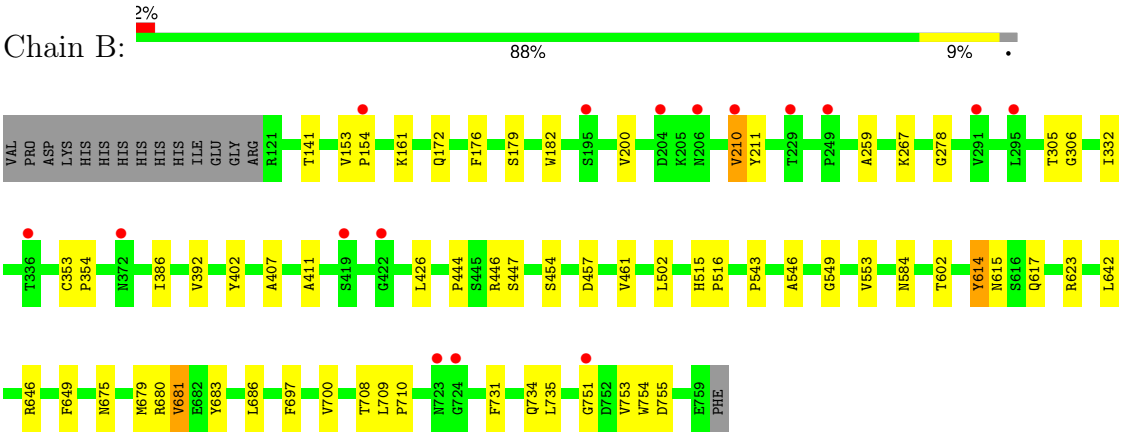
• Molecule 1: Transferrin receptor protein 1

Chain A:



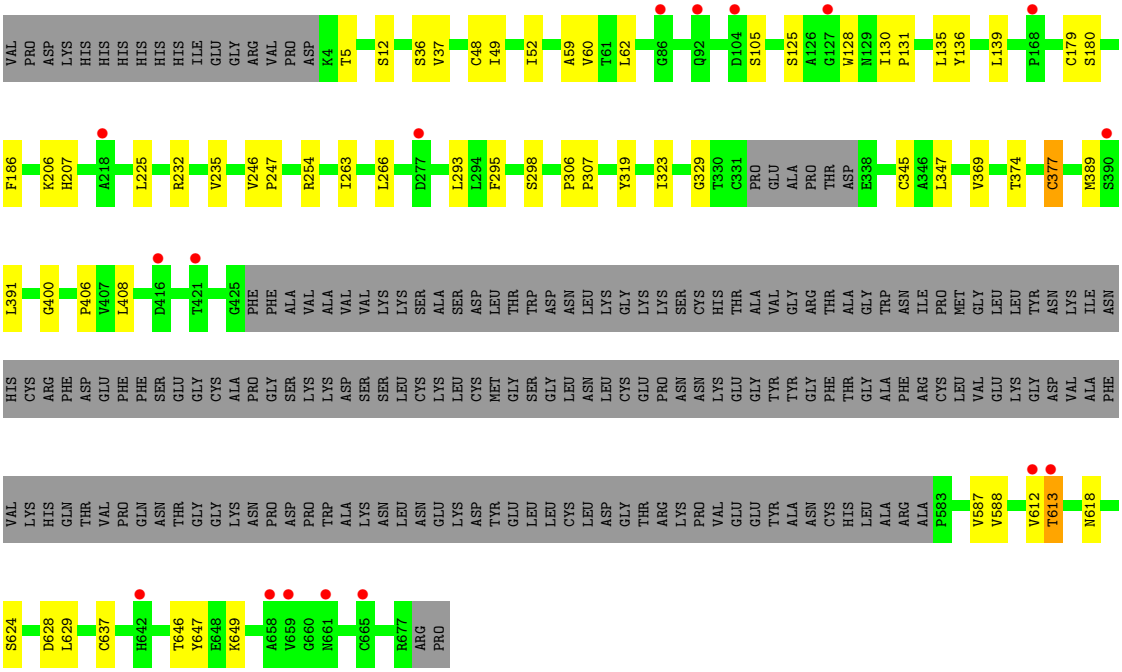
• Molecule 1: Transferrin receptor protein 1

Chain B:



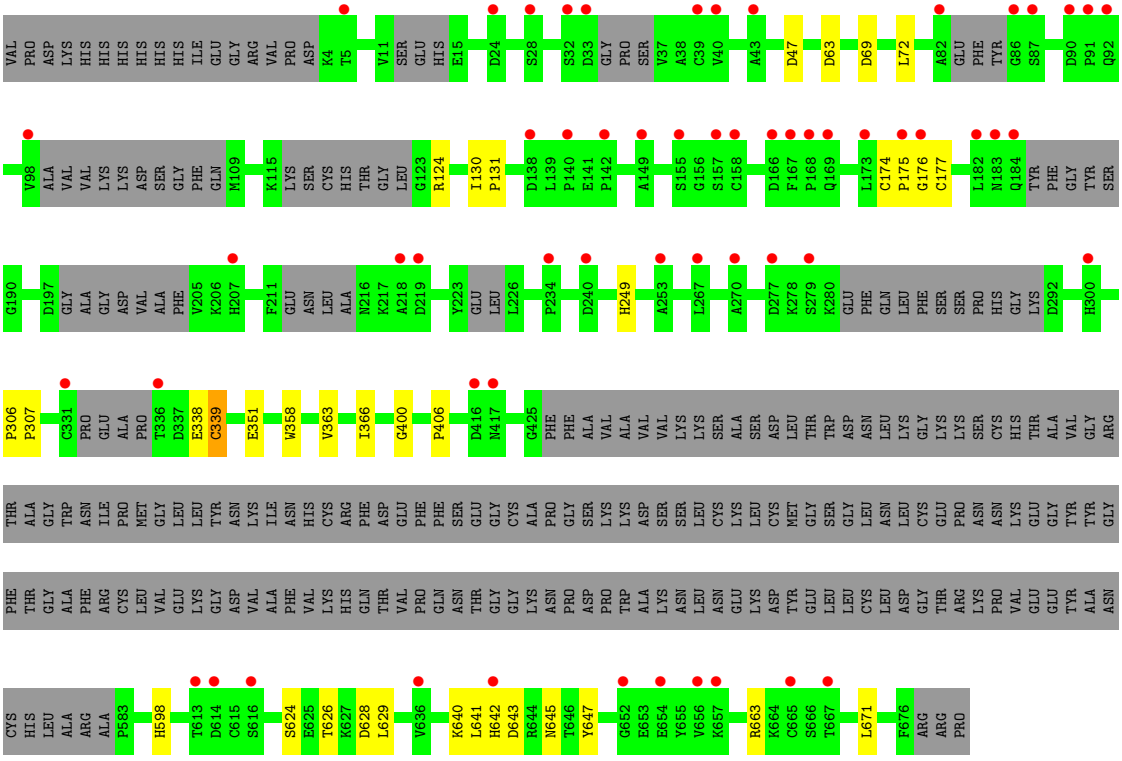
• Molecule 2: Serotransferrin

Chain C:



• Molecule 2: Serotransferrin

Chain D:



4 Data and refinement statistics (i)

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 29.64 – 3.25	Depositor EDS
% Data completeness (in resolution range)	99.3 (30.00-3.25) 99.2 (29.64-3.25)	Depositor EDS
R_{merge}	0.22	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.30 (at 3.24Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.254 , 0.289 0.255 , 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)	0.26 , 74.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: FE, CA, CO3, NAG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.43	0/5036	0.57	0/6860
1	B	0.41	0/4937	0.54	0/6744
2	C	0.35	0/3784	0.50	0/5159
2	D	0.31	0/2854	0.46	1/3913 (0.0%)
All	All	0.39	0/16611	0.53	1/22676 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	47	ASP	CB-CG-OD2	5.22	123.00	118.30

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	107	0
1	B	4820	0	4480	40	0
2	C	3705	0	3318	51	0
2	D	2822	0	2022	32	0
3	A	14	0	13	0	0
3	B	14	0	13	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	228	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 7.

All (228) 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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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: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
1:A:757:ASP:O	1:A:758:ASN:C	2.39	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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
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
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:A:262:ILE:HG23	1:A:266:GLU:CD	2.20	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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: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
2:C:128:TRP:C	2:C:131:PRO:HD2	2.34	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
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:B:680:ARG:O	1:B:681:VAL:C	2.54	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:614:TYR:OH	1:A:702:TRP:CZ3	2.68	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
2:D:641:LEU:O	2:D:642:HIS:CB	2.63	0.45
1:A:262:ILE:CG2	1:A:266:GLU:CD	2.83	0.44
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
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
1:B:444:PRO:HB3	1:B:602:THR:HG21	2.00	0.43
2:D:69:ASP:HA	2:D:72:LEU:HD12	2.00	0.43
1:A:501:LEU:HD23	1:A:610:ASP:C	2.38	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:258:ARG:HH11	1:A:284:ASP:CG	2.22	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:A:614:TYR:OH	1:A:702:TRP:HZ3	2.02	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: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: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
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%)	41	72
1	B	637/654 (97%)	607 (95%)	28 (4%)	2 (0%)	41	72
2	C	505/693 (73%)	474 (94%)	29 (6%)	2 (0%)	34	67
2	D	431/693 (62%)	400 (93%)	29 (7%)	2 (0%)	29	62
All	All	2209/2694 (82%)	2085 (94%)	116 (5%)	8 (0%)	34	67

All (8) Ramachandran outliers are listed below:

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

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%)	512 (100%)	0	100	100
1	B	483/562 (86%)	481 (100%)	2 (0%)	91	94

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	C	366/585 (63%)	364 (100%)	2 (0%)	88 93
2	D	189/585 (32%)	189 (100%)	0	100 100
All	All	1550/2294 (68%)	1546 (100%)	4 (0%)	92 96

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	614	TYR
1	B	646	ARG
2	C	377	CYS
2	C	637	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	148	ASN
1	A	164	ASN
1	A	318	HIS
1	A	320	GLN
1	A	401	HIS
1	A	512	ASN
1	A	596	GLN
1	A	626	ASN
1	A	684	HIS
1	A	734	GLN
1	A	747	ASN
1	A	758	ASN
1	B	148	ASN
1	B	483	ASN
1	B	584	ASN
1	B	596	GLN
1	B	608	ASN
1	B	626	ASN
1	B	734	GLN
1	B	747	ASN
2	C	207	HIS
2	C	349	HIS
2	C	584	ASN
2	C	585	HIS
2	C	604	GLN

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Mol	Chain	Res	Type
2	D	598	HIS
2	D	604	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

There are no monosaccharides in this entry.

5.6 Ligand geometry

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	$\#\|Z\| > 2$
6	CO3	D	905	5	3,3,3	0.28	0	2,3,3	0.21	0
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
3	NAG	B	903	1	14,14,15	0.44	0	17,19,21	1.17	2 (11%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	A	903	1	-	0/6/23/26	0/1/1/1
3	NAG	B	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(^{o})	Ideal(^{o})
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, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	638/654 (97%)	-0.21	10 (1%)	72	69	39, 75, 125, 200	0
1	B	639/654 (97%)	-0.03	16 (2%)	57	53	38, 92, 162, 200	1 (0%)
2	C	511/693 (73%)	0.17	17 (3%)	46	43	65, 112, 172, 200	0
2	D	457/693 (65%)	0.58	58 (12%)	3	3	67, 153, 192, 200	0
All	All	2245/2694 (83%)	0.09	101 (4%)	33	31	38, 100, 179, 200	1 (0%)

All (101) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	724	GLY	7.3
2	D	184	GLN	5.4
2	D	39	CYS	4.7
2	D	149	ALA	4.7
2	D	613	THR	4.5
1	A	722	ASN	4.5
2	D	32	SER	4.4
2	D	28	SER	4.4
2	C	421	THR	4.3
2	D	86	GLY	4.3
2	D	168	PRO	4.3
1	A	195	SER	4.1
2	D	652	GLY	4.1
2	D	176	GLY	4.0
2	D	300	HIS	3.9
1	A	723	ASN	3.9
1	B	751	GLY	3.8
2	D	98	VAL	3.7
2	D	140	PRO	3.6
2	C	613	THR	3.6
2	C	612	VAL	3.6

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Mol	Chain	Res	Type	RSRZ
2	D	642	HIS	3.6
1	B	229	THR	3.6
1	A	721	GLN	3.5
1	A	422	GLY	3.5
2	C	390	SER	3.4
2	C	416	ASP	3.4
2	D	87	SER	3.4
2	C	665	CYS	3.4
2	D	665	CYS	3.3
2	D	33	ASP	3.3
2	D	267	LEU	3.2
2	D	175	PRO	3.2
2	D	138	ASP	3.2
2	C	86	GLY	3.0
1	B	723	ASN	3.0
2	C	92	GLN	3.0
2	C	659	VAL	3.0
2	D	91	PRO	3.0
2	D	656	VAL	2.9
1	B	295	LEU	2.9
1	B	206	ASN	2.9
2	C	168	PRO	2.9
2	D	142	PRO	2.9
2	D	155	SER	2.9
2	D	417	ASN	2.9
2	D	616	SER	2.8
1	A	194	ASP	2.8
2	C	658	ALA	2.8
2	D	90	ASP	2.8
2	C	127	GLY	2.8
2	D	173	LEU	2.8
2	D	207	HIS	2.8
2	D	667	THR	2.8
2	D	614	ASP	2.7
2	D	331	CYS	2.7
2	C	642	HIS	2.7
2	D	167	PHE	2.7
1	B	195	SER	2.6
1	B	422	GLY	2.6
1	B	419	SER	2.6
2	C	218	ALA	2.6
2	D	158	CYS	2.6

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Mol	Chain	Res	Type	RSRZ
2	D	43	ALA	2.6
1	B	210	VAL	2.5
1	B	724	GLY	2.5
1	B	204	ASP	2.5
2	D	218	ALA	2.5
2	D	336	THR	2.5
1	B	372	ASN	2.5
2	D	240	ASP	2.5
1	B	154	PRO	2.4
2	D	416	ASP	2.4
2	D	169	GLN	2.4
1	A	483	ASN	2.4
2	C	661	ASN	2.4
2	D	157	SER	2.3
2	D	270	ALA	2.3
2	C	104	ASP	2.3
2	D	234	PRO	2.3
2	D	40	VAL	2.3
2	D	654	GLU	2.3
2	D	92	GLN	2.3
2	D	253	ALA	2.3
2	D	636	VAL	2.2
2	D	219	ASP	2.2
2	D	82	ALA	2.2
2	C	277	ASP	2.2
2	D	24	ASP	2.2
2	D	5	THR	2.2
1	B	291	VAL	2.2
2	D	182	LEU	2.2
2	D	277	ASP	2.2
1	A	406	GLY	2.2
2	D	166	ASP	2.1
2	D	657	LYS	2.1
2	D	183	ASN	2.1
2	D	279	SER	2.1
1	B	249	PRO	2.1
1	B	336	THR	2.0
1	A	196	ALA	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 monosaccharides 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, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	NAG	B	903	14/15	0.71	0.32	126,126,126,126	0
4	CA	A	900	1/1	0.80	0.20	96,96,96,96	0
3	NAG	A	903	14/15	0.81	0.27	124,124,124,124	0
6	CO3	C	905	4/4	0.83	0.45	96,96,96,96	0
4	CA	B	900	1/1	0.86	0.20	96,96,96,96	0
6	CO3	D	905	4/4	0.88	0.14	96,96,96,96	0
5	FE	C	901	1/1	0.92	0.24	96,96,96,96	0
5	FE	D	901	1/1	0.95	0.05	96,96,96,96	0

6.5 Other polymers (i)

There are no such residues in this entry.