



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:20 AM UTC

PDB ID : 6SOY / pdb_00006soy
Title : Trypanosoma brucei transferrin receptor in complex with human transferrin
Authors : Trevor, C.; Carrington, M.; Higgins, M.K.
Deposited on : 2019-08-30
Resolution : 2.75 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

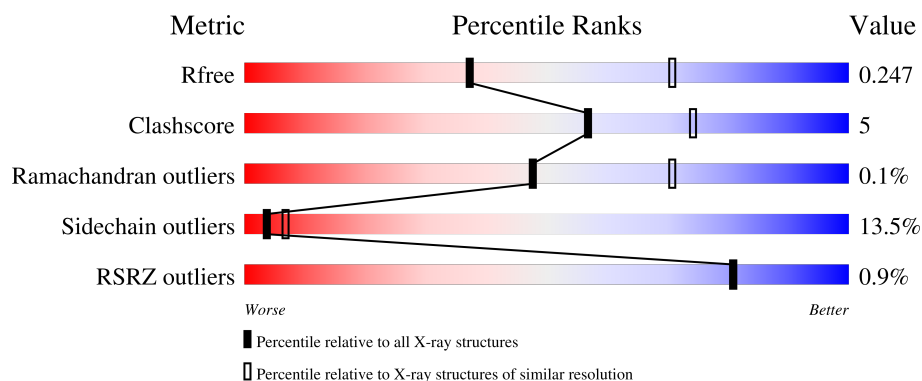
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.75 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	1009 (2.76-2.76)
Clashscore	190562	1044 (2.76-2.76)
Ramachandran outliers	187476	1024 (2.76-2.76)
Sidechain outliers	187428	1024 (2.76-2.76)
RSRZ outliers	180081	1009 (2.76-2.76)

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	399	59% 19% • 19%
2	B	338	2% 70% 18% 5% 7%
3	C	677	77% 17% • •

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 10058 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 ESAG6, subunit of heterodimeric transferrin receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	323	Total	C	N	O	S	0	0	0
			2500	1554	443	492	11			

- Molecule 2 is a protein called ESAG7, subunit of heterodimeric transferrin receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	313	Total	C	N	O	S	0	0	0
			2438	1531	422	473	12			

- Molecule 3 is a protein called Serotransferrin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	652	Total	C	N	O	S	0	0	0
			5067	3187	880	956	44			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	429	VAL	ILE	conflict	UNP P02787

- Molecule 4 is FE (III) ION (CCD ID: FE) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	1	Total	Fe	0	0
			1	1		

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



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

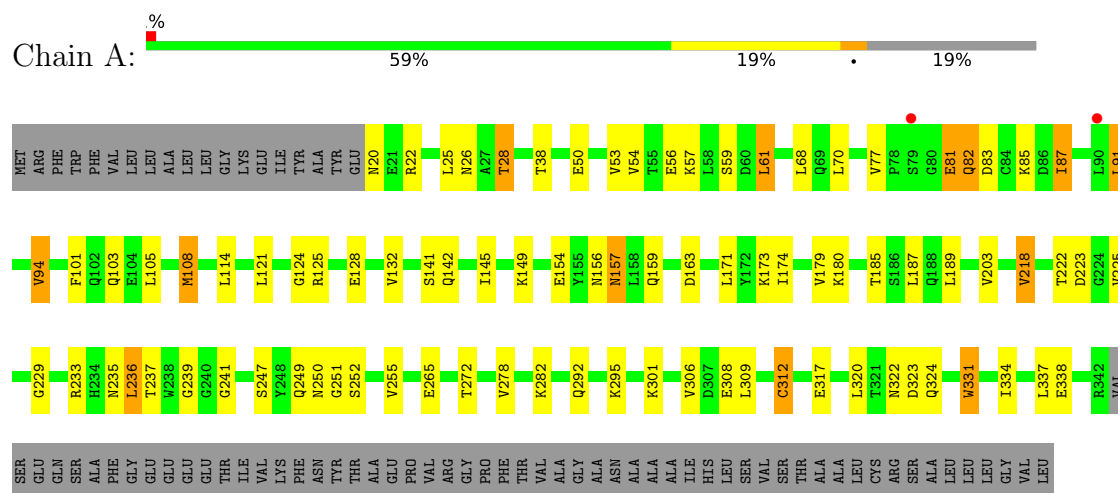
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	13	Total	O	0	0
			13	13		
6	B	6	Total	O	0	0
			6	6		
6	C	19	Total	O	0	0
			19	19		

3 Residue-property plots

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: ESAG6, subunit of heterodimeric transferrin receptor





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	163.49Å 108.11Å 115.00Å 90.00° 128.74° 90.00°	Depositor
Resolution (Å)	40.26 – 2.75 40.26 – 2.75	Depositor EDS
% Data completeness (in resolution range)	98.9 (40.26-2.75) 98.8 (40.26-2.75)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.59 (at 2.77Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, R_{free}	0.183 , 0.233 0.193 , 0.247	Depositor DCC
R_{free} test set	2014 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	68.1	Xtriage
Anisotropy	0.455	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 72.6	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	0.95	EDS
Total number of atoms	10058	wwPDB-VP
Average B, all atoms (Å ²)	79.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.04% 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: FE, 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	0.92	1/2535 (0.0%)	1.55	26/3414 (0.8%)
2	B	0.90	0/2472	1.48	12/3328 (0.4%)
3	C	0.88	0/5181	1.40	32/6998 (0.5%)
All	All	0.89	1/10188 (0.0%)	1.46	70/13740 (0.5%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	218	VAL	CA-C	5.67	1.59	1.52

All (70) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	157	ASN	N-CA-C	-8.20	99.96	110.53
1	A	218	VAL	N-CA-CB	-7.24	102.75	112.16
1	A	239	GLY	N-CA-C	-6.21	101.42	112.22
1	A	322	ASN	CA-C-N	6.13	128.49	120.28
1	A	322	ASN	C-N-CA	6.13	128.49	120.28
1	A	82	GLN	N-CA-C	-6.12	100.37	109.86
3	C	589	THR	CA-C-N	6.05	129.35	120.82
3	C	589	THR	C-N-CA	6.05	129.35	120.82
1	A	251	GLY	N-CA-C	-5.98	106.38	115.00
2	B	121	ILE	N-CA-CB	5.91	117.46	110.55
1	A	124	GLY	CA-C-N	5.87	128.07	120.44
1	A	124	GLY	C-N-CA	5.87	128.07	120.44
3	C	105	SER	CA-C-N	5.83	128.92	120.11
3	C	105	SER	C-N-CA	5.83	128.92	120.11
3	C	26	MET	CA-C-N	5.83	128.89	120.38
3	C	26	MET	C-N-CA	5.83	128.89	120.38
2	B	254	ILE	N-CA-CB	5.78	117.42	110.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	237	GLU	CA-C-N	5.74	128.76	120.38
3	C	237	GLU	C-N-CA	5.74	128.76	120.38
3	C	573	GLU	CA-C-N	5.73	127.96	120.28
3	C	573	GLU	C-N-CA	5.73	127.96	120.28
3	C	481	SER	N-CA-C	-5.72	104.68	111.03
2	B	238	GLY	N-CA-C	-5.71	102.28	112.22
3	C	31	PRO	CA-C-N	5.67	128.15	120.38
3	C	31	PRO	C-N-CA	5.67	128.15	120.38
3	C	120	THR	N-CA-C	-5.67	104.79	110.97
1	A	249	GLN	CA-C-N	5.65	130.18	121.19
1	A	249	GLN	C-N-CA	5.65	130.18	121.19
1	A	20	ASN	CA-CB-CG	5.62	118.22	112.60
3	C	460	TRP	CA-C-N	5.61	128.06	120.38
3	C	460	TRP	C-N-CA	5.61	128.06	120.38
1	A	223	ASP	CA-CB-CG	5.59	118.19	112.60
3	C	131	PRO	CA-C-N	5.44	127.92	120.46
3	C	131	PRO	C-N-CA	5.44	127.92	120.46
2	B	230	CYS	N-CA-C	-5.43	103.36	110.53
2	B	106	GLU	CA-C-N	5.43	127.55	120.28
2	B	106	GLU	C-N-CA	5.43	127.55	120.28
3	C	290	GLY	N-CA-C	5.42	117.41	110.96
1	A	272	THR	N-CA-C	5.35	118.10	110.24
2	B	84	CYS	CA-C-N	5.33	131.72	121.54
2	B	84	CYS	C-N-CA	5.33	131.72	121.54
3	C	529	ASP	CA-CB-CG	5.33	117.93	112.60
3	C	325	ASN	CA-CB-CG	5.33	117.93	112.60
3	C	348	SER	CA-C-N	5.29	127.90	120.28
3	C	348	SER	C-N-CA	5.29	127.90	120.28
3	C	106	GLY	N-CA-C	5.26	121.15	113.48
3	C	396	VAL	N-CA-C	-5.25	105.60	110.53
1	A	173	LYS	CA-C-N	5.19	127.85	120.53
1	A	173	LYS	C-N-CA	5.19	127.85	120.53
1	A	179	VAL	CA-C-N	5.18	127.23	120.28
1	A	179	VAL	C-N-CA	5.18	127.23	120.28
2	B	272	GLU	N-CA-C	-5.18	107.09	113.41
2	B	272	GLU	CB-CG-CD	5.18	121.40	112.60
1	A	235	ASN	CA-CB-CG	5.17	117.77	112.60
1	A	81	GLU	N-CA-C	-5.14	103.69	111.56
1	A	278	VAL	CA-C-N	5.12	128.50	120.82
1	A	278	VAL	C-N-CA	5.12	128.50	120.82
1	A	331	TRP	CA-C-N	5.10	127.53	120.29
1	A	331	TRP	C-N-CA	5.10	127.53	120.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	193	LYS	CA-C-N	5.10	127.11	120.28
3	C	193	LYS	C-N-CA	5.10	127.11	120.28
1	A	56	GLU	CA-C-N	5.07	127.07	120.28
1	A	56	GLU	C-N-CA	5.07	127.07	120.28
3	C	313	MET	CA-C-N	5.05	127.01	120.44
3	C	313	MET	C-N-CA	5.05	127.01	120.44
3	C	38	ALA	CA-C-N	-5.05	114.74	122.87
3	C	38	ALA	C-N-CA	-5.05	114.74	122.87
2	B	20	ASN	CA-CB-CG	5.05	117.65	112.60
2	B	23	ASN	CA-CB-CG	5.04	117.64	112.60
3	C	246	VAL	N-CA-C	5.00	115.62	107.71

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2500	0	2474	28	0
2	B	2438	0	2420	33	0
3	C	5067	0	4913	40	0
4	C	1	0	0	0	0
5	C	14	0	13	0	0
6	A	13	0	0	0	0
6	B	6	0	0	0	0
6	C	19	0	0	0	0
All	All	10058	0	9820	92	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 5.

All (92) 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)
3:C:538:VAL:HB	3:C:571:VAL:HG11	1.67	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:319:LEU:HB3	2:B:324:LEU:HD12	1.72	0.72
2:B:257:GLY:HA3	2:B:269:ARG:HG2	1.69	0.72
1:A:154:GLU:H	1:A:157:ASN:HD22	1.36	0.71
1:A:331:TRP:HD1	2:B:88:ARG:NH2	1.89	0.70
3:C:383:ASN:HD21	3:C:385:GLU:HG3	1.59	0.68
1:A:94:VAL:HG21	1:A:309:LEU:HD21	1.75	0.67
1:A:26:ASN:ND2	1:A:28:THR:HG22	2.10	0.66
3:C:605:GLN:HE21	3:C:637:CYS:HB2	1.62	0.65
1:A:233:ARG:HG3	2:B:139:GLY:H	1.62	0.65
3:C:604:GLN:HE22	3:C:608:PHE:HD2	1.45	0.64
1:A:331:TRP:HD1	2:B:88:ARG:HH22	1.44	0.64
1:A:26:ASN:HD22	1:A:28:THR:HG22	1.62	0.62
3:C:37:VAL:HG22	3:C:266:LEU:HD11	1.82	0.61
1:A:237:THR:OG1	1:A:241:GLY:HA2	2.00	0.60
3:C:397:TYR:HE1	3:C:656:VAL:HG13	1.65	0.60
2:B:25:LEU:N	2:B:218:MET:HE1	2.18	0.59
3:C:358:TRP:HE1	3:C:604:GLN:NE2	2.01	0.58
1:A:25:LEU:O	1:A:145:ILE:HA	2.03	0.57
2:B:178:ARG:HA	2:B:181:GLU:HG2	1.87	0.56
1:A:108:MET:HE2	1:A:295:LYS:HA	1.87	0.56
1:A:54:VAL:HG11	1:A:108:MET:HE1	1.89	0.55
3:C:440:THR:HG22	3:C:442:ASP:H	1.72	0.55
1:A:50:GLU:HB3	1:A:295:LYS:HE2	1.90	0.54
3:C:259:LYS:HB3	3:C:262:LEU:HB3	1.89	0.54
2:B:154:GLU:H	2:B:157:ASN:HD22	1.56	0.53
2:B:257:GLY:CA	2:B:269:ARG:HG2	2.38	0.53
3:C:233:LYS:HD2	3:C:241:CYS:HB2	1.89	0.53
3:C:210:ILE:HD13	3:C:235:VAL:HG11	1.89	0.53
1:A:114:LEU:HD22	2:B:174:ILE:HD11	1.91	0.53
3:C:395:PHE:HE2	3:C:456:ARG:HG2	1.74	0.53
2:B:54:VAL:HG21	2:B:108:MET:HE1	1.91	0.53
2:B:323:GLN:HE21	2:B:323:GLN:H	1.55	0.52
3:C:600:ILE:O	3:C:604:GLN:HB2	2.08	0.52
1:A:101:PHE:HE1	1:A:301:LYS:HE2	1.76	0.51
2:B:162:PHE:HD1	2:B:170:THR:HG23	1.75	0.51
3:C:453:ALA:HB3	3:C:456:ARG:HG3	1.92	0.50
3:C:605:GLN:NE2	3:C:637:CYS:HB2	2.27	0.50
2:B:154:GLU:H	2:B:157:ASN:ND2	2.10	0.50
1:A:82:GLN:HG3	1:A:83:ASP:H	1.77	0.48
1:A:250:ASN:HB3	1:A:252:SER:H	1.78	0.48
3:C:524:LEU:HB2	3:C:531:ALA:HB2	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:499:MET:HE2	3:C:513:GLY:HA3	1.96	0.48
2:B:70:LEU:HD21	2:B:327:GLU:HB3	1.97	0.47
3:C:121:GLY:HA2	3:C:160:PRO:HD2	1.96	0.47
1:A:132:VAL:HG13	2:B:235:PHE:HZ	1.79	0.47
2:B:254:ILE:HG23	2:B:268:VAL:HG12	1.96	0.47
3:C:487:GLY:HA2	3:C:508:PRO:HG3	1.95	0.47
2:B:67:GLN:HG3	2:B:324:LEU:HD11	1.97	0.47
3:C:371:ALA:HB3	3:C:377:CYS:SG	2.55	0.46
1:A:236:LEU:HD22	2:B:135:GLN:HB2	1.98	0.46
3:C:29:VAL:HG23	3:C:30:ILE:HD12	1.97	0.46
3:C:457:THR:HG22	3:C:462:ILE:HD12	1.97	0.46
1:A:229:GLY:HA3	2:B:142:GLN:HG3	1.98	0.46
3:C:361:ASN:HB3	3:C:608:PHE:CZ	2.51	0.45
2:B:72:VAL:HG11	2:B:91:LEU:HD11	1.98	0.45
2:B:153:ALA:HA	2:B:157:ASN:HD22	1.81	0.45
2:B:309:THR:HA	2:B:312:ILE:HD12	1.98	0.45
1:A:68:LEU:HD22	1:A:309:LEU:HD22	1.98	0.44
1:A:237:THR:H	2:B:135:GLN:HE22	1.65	0.44
2:B:21:GLU:HA	2:B:212:ASN:ND2	2.33	0.44
3:C:109:MET:HE3	3:C:228:LEU:HD23	1.99	0.44
1:A:54:VAL:HG21	1:A:295:LYS:HG2	2.00	0.44
3:C:433:LYS:HE3	3:C:524:LEU:HD11	2.00	0.44
2:B:252:LEU:HG	2:B:268:VAL:HG21	2.00	0.44
1:A:128:GLU:OE1	2:B:125:ARG:HD2	2.18	0.44
1:A:26:ASN:HD22	1:A:28:THR:H	1.66	0.43
2:B:173:LYS:O	2:B:176:ASP:HB2	2.17	0.43
3:C:447:LYS:HB3	3:C:529:ASP:OD1	2.18	0.43
1:A:77:VAL:HG13	1:A:312:CYS:HB3	1.99	0.43
1:A:247:SER:OG	1:A:265:GLU:HG2	2.19	0.43
3:C:18:LYS:HE3	3:C:287:SER:HB2	1.99	0.43
2:B:165:THR:O	2:B:170:THR:HG21	2.19	0.43
3:C:347:LEU:HD23	3:C:347:LEU:HA	1.84	0.43
3:C:227:CYS:HB2	3:C:229:ASP:OD1	2.19	0.42
2:B:118:ALA:HA	2:B:121:ILE:HD12	2.02	0.42
2:B:262:VAL:HG13	2:B:267:ALA:HB3	2.01	0.42
3:C:35:PRO:HG3	3:C:265:GLU:HG2	2.02	0.42
1:A:87:ILE:O	1:A:91:LEU:HB2	2.20	0.42
3:C:518:THR:HG23	3:C:541:ASN:OD1	2.20	0.42
3:C:475:ARG:HH11	3:C:478:GLU:HG2	1.86	0.41
2:B:109:ARG:HA	2:B:109:ARG:HD2	1.90	0.41
3:C:407:VAL:HG11	3:C:594:GLU:HA	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:23:ARG:HH11	3:C:39:CYS:H	1.68	0.41
3:C:310:ASP:OD1	3:C:313:MET:HB2	2.20	0.41
3:C:392:ASP:HA	3:C:585:HIS:CD2	2.55	0.41
1:A:61:LEU:HD23	1:A:306:VAL:HG23	2.03	0.41
2:B:252:LEU:HB3	2:B:254:ILE:CD1	2.50	0.41
3:C:287:SER:HB3	3:C:293:LEU:HD12	2.03	0.41
3:C:107:PHE:H	3:C:232:ARG:NH2	2.18	0.40
3:C:377:CYS:HB3	3:C:389:MET:SD	2.60	0.40
3:C:644:ARG:HA	3:C:649:LYS:HB3	2.03	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	321/399 (80%)	301 (94%)	20 (6%)	0	100	100
2	B	309/338 (91%)	291 (94%)	18 (6%)	0	100	100
3	C	646/677 (95%)	602 (93%)	43 (7%)	1 (0%)	43	64
All	All	1276/1414 (90%)	1194 (94%)	81 (6%)	1 (0%)	48	71

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	363	VAL

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	268/327 (82%)	221 (82%)	47 (18%)	2	3
2	B	262/283 (93%)	219 (84%)	43 (16%)	2	3
3	C	548/570 (96%)	493 (90%)	55 (10%)	7	14
All	All	1078/1180 (91%)	933 (86%)	145 (14%)	4	7

All (145) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	ARG
1	A	28	THR
1	A	38	THR
1	A	53	VAL
1	A	57	LYS
1	A	59	SER
1	A	61	LEU
1	A	70	LEU
1	A	81	GLU
1	A	85	LYS
1	A	87	ILE
1	A	91	LEU
1	A	94	VAL
1	A	103	GLN
1	A	105	LEU
1	A	108	MET
1	A	121	LEU
1	A	125	ARG
1	A	141	SER
1	A	142	GLN
1	A	149	LYS
1	A	156	ASN
1	A	159	GLN
1	A	163	ASP
1	A	171	LEU
1	A	174	ILE
1	A	180	LYS
1	A	185	THR
1	A	187	LEU
1	A	189	LEU
1	A	203	VAL

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Mol	Chain	Res	Type
1	A	218	VAL
1	A	222	THR
1	A	225	VAL
1	A	236	LEU
1	A	255	VAL
1	A	282	LYS
1	A	292	GLN
1	A	308	GLU
1	A	312	CYS
1	A	317	GLU
1	A	320	LEU
1	A	323	ASP
1	A	324	GLN
1	A	334	ILE
1	A	337	LEU
1	A	338	GLU
2	B	20	ASN
2	B	22	ARG
2	B	25	LEU
2	B	32	LYS
2	B	63	MET
2	B	70	LEU
2	B	72	VAL
2	B	85	LYS
2	B	108	MET
2	B	125	ARG
2	B	141	SER
2	B	142	GLN
2	B	158	LEU
2	B	159	GLN
2	B	169	GLU
2	B	170	THR
2	B	174	ILE
2	B	176	ASP
2	B	177	SER
2	B	189	LEU
2	B	196	ILE
2	B	201	LEU
2	B	205	SER
2	B	207	VAL
2	B	211	GLU
2	B	213	ARG

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Mol	Chain	Res	Type
2	B	226	LEU
2	B	227	LYS
2	B	242	LEU
2	B	253	LYS
2	B	254	ILE
2	B	266	ASP
2	B	269	ARG
2	B	272	GLU
2	B	282	ASP
2	B	289	ARG
2	B	300	LYS
2	B	314	GLN
2	B	319	LEU
2	B	323	GLN
2	B	324	LEU
2	B	331	ILE
2	B	337	PHE
3	C	17	THR
3	C	27	LYS
3	C	28	SER
3	C	30	ILE
3	C	37	VAL
3	C	39	CYS
3	C	42	LYS
3	C	46	LEU
3	C	50	ARG
3	C	55	ASN
3	C	61	THR
3	C	71	TYR
3	C	144	LYS
3	C	172	GLN
3	C	182	LEU
3	C	217	LYS
3	C	227	CYS
3	C	249	HIS
3	C	250	THR
3	C	256	MET
3	C	259	LYS
3	C	280	LYS
3	C	284	LEU
3	C	286	SER
3	C	291	LYS

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Mol	Chain	Res	Type
3	C	304	LYS
3	C	330	THR
3	C	343	LYS
3	C	347	LEU
3	C	353	LEU
3	C	372	GLU
3	C	383	ASN
3	C	389	MET
3	C	416	ASP
3	C	419	GLU
3	C	433	LYS
3	C	445	LYS
3	C	454	VAL
3	C	456	ARG
3	C	470	LYS
3	C	478	GLU
3	C	488	SER
3	C	503	LEU
3	C	540	GLN
3	C	548	ASP
3	C	553	ASN
3	C	560	GLU
3	C	576	ASN
3	C	588	VAL
3	C	592	ASP
3	C	599	LYS
3	C	604	GLN
3	C	627	LYS
3	C	646	THR
3	C	664	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	ASN
1	A	26	ASN
1	A	67	GLN
1	A	82	GLN
1	A	102	GLN
1	A	157	ASN
1	A	234	HIS
1	A	235	ASN

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Mol	Chain	Res	Type
2	B	26	ASN
2	B	135	GLN
2	B	150	ASN
2	B	157	ASN
2	B	321	ASN
2	B	323	GLN
3	C	55	ASN
3	C	76	ASN
3	C	110	ASN
3	C	172	GLN
3	C	184	GLN
3	C	222	GLN
3	C	289	HIS
3	C	350	HIS
3	C	383	ASN
3	C	417	ASN
3	C	540	GLN
3	C	546	ASN
3	C	603	GLN
3	C	604	GLN
3	C	605	GLN
3	C	645	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 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
5	NAG	C	702	3	14,14,15	0.31	0	17,19,21	1.09	1 (5%)

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
5	NAG	C	702	3	-	1/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	702	NAG	C1-O5-C5	3.75	117.21	112.19

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	702	NAG	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	323/399 (80%)	-0.09	2 (0%) 85 86	45, 66, 132, 153	0
2	B	313/338 (92%)	0.04	6 (1%) 66 64	47, 71, 124, 143	0
3	C	652/677 (96%)	-0.05	3 (0%) 87 87	47, 78, 105, 125	0
All	All	1288/1414 (91%)	-0.04	11 (0%) 81 81	45, 74, 118, 153	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	39	CYS	3.4
2	B	138	GLY	3.0
2	B	72	VAL	2.7
2	B	73	MET	2.6
1	A	90	LEU	2.3
2	B	87	ILE	2.3
1	A	79	SER	2.3
3	C	332	PRO	2.2
3	C	330	THR	2.1
2	B	334	TYR	2.1
2	B	177	SER	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	NAG	C	702	14/15	0.63	0.14	141,144,146,147	0
4	FE	C	701	1/1	0.92	0.12	77,77,77,77	0

6.5 Other polymers [i](#)

There are no such residues in this entry.