Full wwPDB X-ray Structure Validation Report ⓘ

Aug 8, 2020 – 11:19 PM BST

PDB ID	:	6SOY
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 following versions of software and data (see references ⓘ) were used in the production of this report:

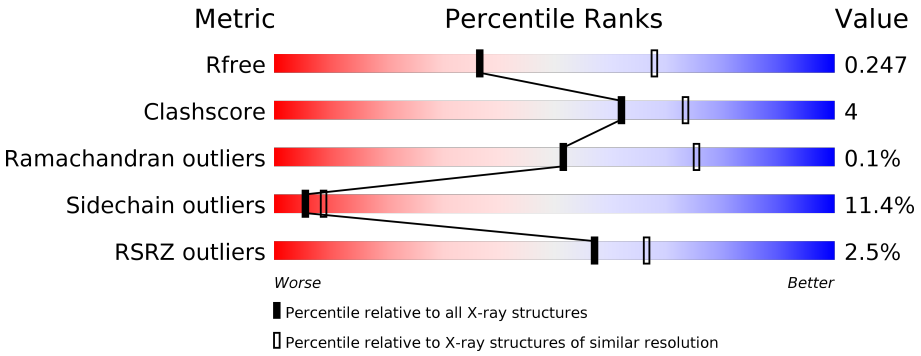
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

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 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}	130704	1235 (2.78-2.74)
Clashscore	141614	1277 (2.78-2.74)
Ramachandran outliers	138981	1257 (2.78-2.74)
Sidechain outliers	138945	1257 (2.78-2.74)
RSRZ outliers	127900	1207 (2.78-2.74)

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 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	399	3% 64% 15% • 19%
2	B	338	3% 72% 17% • 7%
3	C	677	% 81% 14% • •

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			

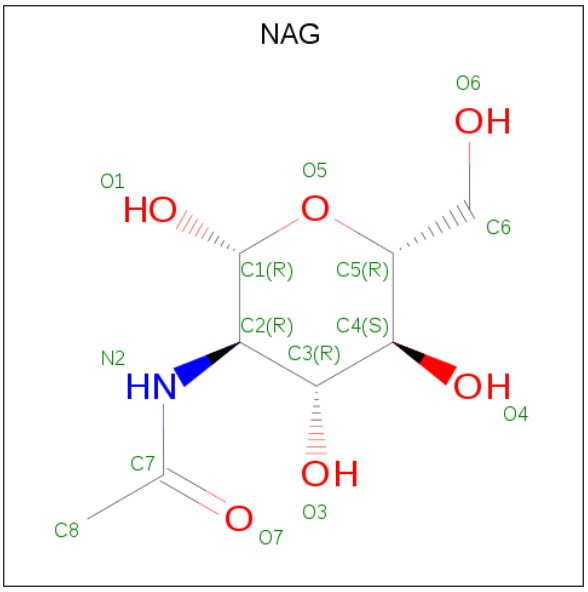
There is a discrepancy between the modelled and reference sequences:

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

- Molecule 4 is FE (III) ION (three-letter code: 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 (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

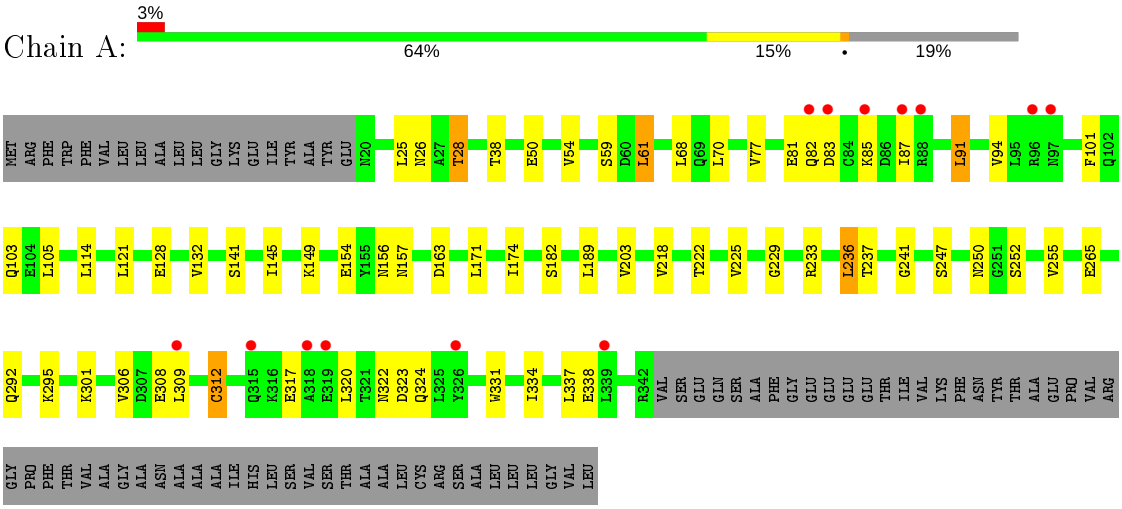
- Molecule 6 is water.

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

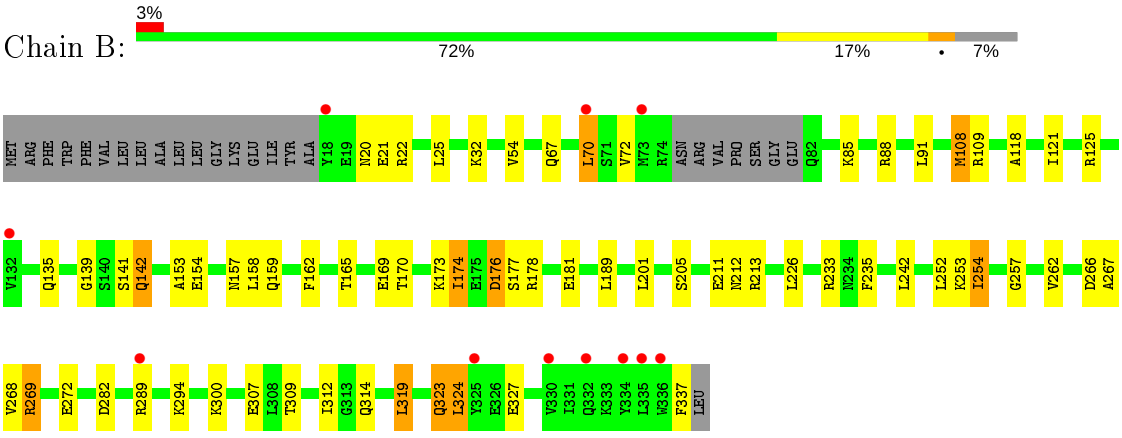
3 Residue-property plots (i)

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.

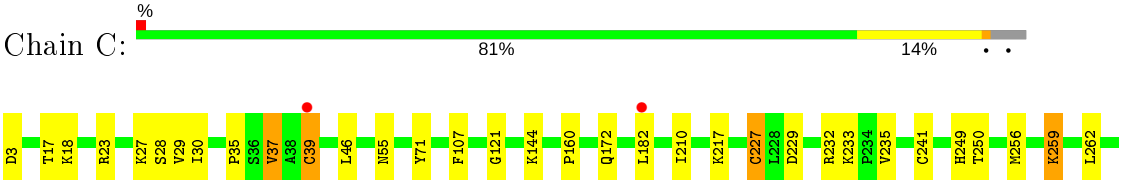
• Molecule 1: ESAG6, subunit of heterodimeric transferrin receptor

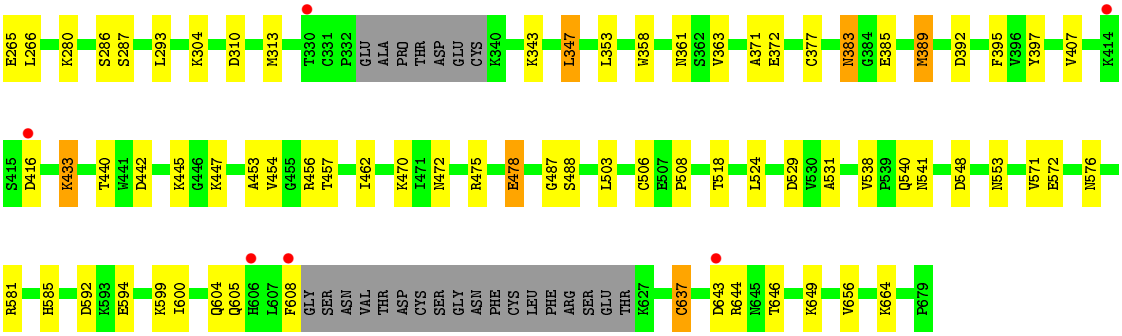


• Molecule 2: ESAG7, subunit of heterodimeric transferrin receptor



• Molecule 3: Serotransferrin




E265 L266 K280 S286 S287 L293 K304 D310 M313 T330 C331 P332 GLU ALA PRO THR ASP GLU CYS K340 K343 L347 L353 W358 N361 S362 V363 A371 E372 C377 N383 G384 E385 M389 D392 F395 V396 Y397 V407 K414
S415 D416 K433 T440 W441 D442 K445 G446 K447 A453 V454 G455 R456 T457 I462 K470 I471 N472 R475 E478 G487 S488 L503 C506 E507 P508 T518 L524 D529 V530 A531 V538 P539 Q540 N541 D548 N553 V571 E572 N576
R581 H585 D592 K593 E594 K599 I600 Q604 Q605 H606 L607 F608 GLY SER ASN VAL THR ASP CYS SER GLY ASN PHE CYS LEU PHE ARG SER GLU THR K627 C637 D643 R644 M645 T646 K649 V656 K664 P679

4 Data and refinement statistics (i)

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 39.56 – 2.75	Depositor EDS
% Data completeness (in resolution range)	98.9 (40.26-2.75) 98.9 (39.56-2.75)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [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 , 60.5	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	0.95	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.*

[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: NAG, FE

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	0/2535	0.75	0/3414
2	B	0.51	0/2472	0.75	0/3328
3	C	0.51	0/5181	0.71	0/6998
All	All	0.51	0/10188	0.73	0/13740

There are no bond length outliers.

There are no bond angle outliers.

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	2500	0	2474	27	0
2	B	2438	0	2420	32	0
3	C	5067	0	4913	38	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	88	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 4.

All (88) 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
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
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
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: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:237:THR:HG1	1:A:241:GLY:HA2	1.74	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:524:LEU:HB2	3:C:531:ALA:HB2	1.94	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
2:B:54:VAL:HG21	2:B:108:MET:HE1	1.99	0.45
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
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:HD2	2:B:109:ARG:HA	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%)	47	69
All	All	1276/1414 (90%)	1194 (94%)	81 (6%)	1 (0%)	51	75

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%)	232 (87%)	36 (13%)	4 5
2	B	262/283 (93%)	224 (86%)	38 (14%)	3 4
3	C	548/570 (96%)	499 (91%)	49 (9%)	9 17
All	All	1078/1180 (91%)	955 (89%)	123 (11%)	5 9

All (123) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	THR
1	A	38	THR
1	A	59	SER
1	A	61	LEU
1	A	70	LEU
1	A	81	GLU
1	A	85	LYS
1	A	91	LEU
1	A	103	GLN
1	A	105	LEU
1	A	121	LEU
1	A	141	SER
1	A	149	LYS
1	A	156	ASN
1	A	163	ASP
1	A	171	LEU
1	A	174	ILE
1	A	182	SER
1	A	189	LEU
1	A	203	VAL
1	A	218	VAL
1	A	222	THR
1	A	225	VAL
1	A	236	LEU
1	A	255	VAL
1	A	292	GLN
1	A	308	GLU
1	A	312	CYS
1	A	317	GLU
1	A	320	LEU
1	A	322	ASN

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Mol	Chain	Res	Type
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	70	LEU
2	B	85	LYS
2	B	108	MET
2	B	141	SER
2	B	142	GLN
2	B	158	LEU
2	B	159	GLN
2	B	169	GLU
2	B	174	ILE
2	B	176	ASP
2	B	177	SER
2	B	189	LEU
2	B	201	LEU
2	B	205	SER
2	B	211	GLU
2	B	213	ARG
2	B	226	LEU
2	B	233	ARG
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	294	LYS
2	B	300	LYS
2	B	307	GLU
2	B	314	GLN
2	B	319	LEU
2	B	323	GLN
2	B	324	LEU

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Mol	Chain	Res	Type
2	B	337	PHE
3	C	3	ASP
3	C	17	THR
3	C	27	LYS
3	C	28	SER
3	C	37	VAL
3	C	39	CYS
3	C	46	LEU
3	C	55	ASN
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	286	SER
3	C	304	LYS
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	433	LYS
3	C	445	LYS
3	C	454	VAL
3	C	470	LYS
3	C	472	ASN
3	C	478	GLU
3	C	488	SER
3	C	503	LEU
3	C	506	CYS
3	C	540	GLN
3	C	548	ASP
3	C	553	ASN
3	C	572	GLU

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Mol	Chain	Res	Type
3	C	576	ASN
3	C	581	ARG
3	C	592	ASP
3	C	599	LYS
3	C	637	CYS
3	C	643	ASP
3	C	646	THR
3	C	664	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	ASN
1	A	26	ASN
1	A	157	ASN
1	A	234	HIS
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	383	ASN
3	C	584	ASN
3	C	603	GLN
3	C	604	GLN
3	C	605	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 (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	0.30	0	17,19,21	1.07	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(^{o})	Ideal(^{o})
5	C	702	NAG	C1-O5-C5	3.71	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

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	323/399 (80%)	0.00	13 (4%) 38 45	45, 66, 132, 153	0
2	B	313/338 (92%)	0.01	11 (3%) 44 52	47, 71, 124, 143	0
3	C	652/677 (96%)	-0.14	8 (1%) 79 85	47, 78, 105, 125	0
All	All	1288/1414 (91%)	-0.07	32 (2%) 57 66	45, 74, 118, 153	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	339	LEU	4.6
3	C	414	LYS	3.9
3	C	330	THR	3.4
1	A	315	GLN	3.2
2	B	336	TRP	3.2
2	B	334	TYR	3.1
1	A	326	TYR	3.0
1	A	87	ILE	2.9
2	B	325	TYR	2.9
2	B	332	GLN	2.8
1	A	85	LYS	2.7
1	A	88	ARG	2.7
3	C	416	ASP	2.7
3	C	39	CYS	2.6
1	A	82	GLN	2.5
3	C	606	HIS	2.4
1	A	96	ARG	2.4
1	A	97	ASN	2.3
2	B	18	TYR	2.3
3	C	608	PHE	2.3
2	B	335	LEU	2.3
2	B	132	VAL	2.2
2	B	330	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
2	B	70	LEU	2.2
1	A	319	GLU	2.1
1	A	83	ASP	2.1
2	B	73	MET	2.1
3	C	182	LEU	2.1
1	A	318	ALA	2.1
3	C	643	ASP	2.0
1	A	309	LEU	2.0
2	B	289	ARG	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
5	NAG	C	702	14/15	0.80	0.28	141,144,146,147	0
4	FE	C	701	1/1	0.97	0.26	77,77,77,77	0

6.5 Other polymers (i)

There are no such residues in this entry.