



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 9, 2020 – 08:23 PM BST

PDB ID : 6OKD
Title : Crystal Structure of human transferrin receptor in complex with a cystine-dense peptide
Authors : Finton, K.A.K.; Rupert, P.B.; Strong, R.K.
Deposited on : 2019-04-12
Resolution : 1.85 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

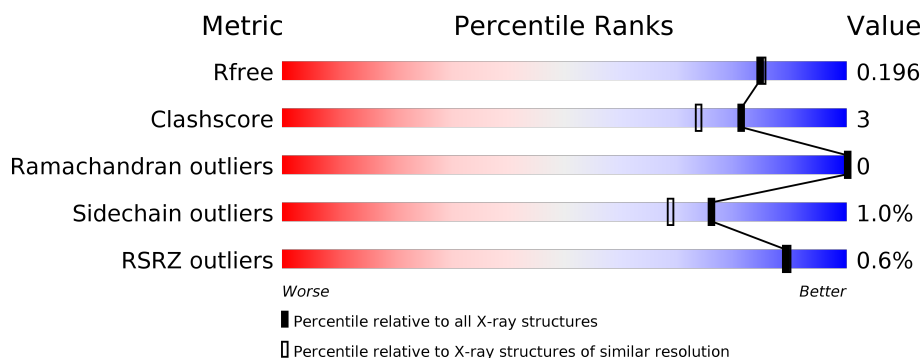
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.85 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	2469 (1.86-1.86)
Clashscore	141614	2625 (1.86-1.86)
Ramachandran outliers	138981	2592 (1.86-1.86)
Sidechain outliers	138945	2592 (1.86-1.86)
RSRZ outliers	127900	2436 (1.86-1.86)

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 $\leq 5\%$. 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	670	 87% 5% 8%
1	B	670	 86% 6% 8%
2	C	51	 6% 84% 16%
2	D	51	 2% 82% 18%

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	GOL	A	703	-	-	X	-

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 11117 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	619	Total	C	N	O	S	0	5	0
			4792	3083	793	902	14			
1	B	617	Total	C	N	O	S	0	5	0
			4776	3075	792	895	14			

There are 62 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	expression tag	UNP P02786
A	2	SER	-	expression tag	UNP P02786
A	24	SER	GLY	conflict	UNP P02786
A	643	GLY	-	expression tag	UNP P02786
A	644	GLY	-	expression tag	UNP P02786
A	645	GLY	-	expression tag	UNP P02786
A	646	SER	-	expression tag	UNP P02786
A	647	HIS	-	expression tag	UNP P02786
A	648	HIS	-	expression tag	UNP P02786
A	649	HIS	-	expression tag	UNP P02786
A	650	HIS	-	expression tag	UNP P02786
A	651	HIS	-	expression tag	UNP P02786
A	652	HIS	-	expression tag	UNP P02786
A	653	GLY	-	expression tag	UNP P02786
A	654	GLY	-	expression tag	UNP P02786
A	655	GLY	-	expression tag	UNP P02786
A	656	SER	-	expression tag	UNP P02786
A	657	LEU	-	expression tag	UNP P02786
A	658	ASN	-	expression tag	UNP P02786
A	659	ASP	-	expression tag	UNP P02786
A	660	ILE	-	expression tag	UNP P02786
A	661	PHE	-	expression tag	UNP P02786
A	662	GLU	-	expression tag	UNP P02786
A	663	ALA	-	expression tag	UNP P02786
A	664	GLN	-	expression tag	UNP P02786

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Chain	Residue	Modelled	Actual	Comment	Reference
A	665	LYS	-	expression tag	UNP P02786
A	666	ILE	-	expression tag	UNP P02786
A	667	GLU	-	expression tag	UNP P02786
A	668	TRP	-	expression tag	UNP P02786
A	669	HIS	-	expression tag	UNP P02786
A	670	GLU	-	expression tag	UNP P02786
B	1	GLY	-	expression tag	UNP P02786
B	2	SER	-	expression tag	UNP P02786
B	24	SER	GLY	conflict	UNP P02786
B	643	GLY	-	expression tag	UNP P02786
B	644	GLY	-	expression tag	UNP P02786
B	645	GLY	-	expression tag	UNP P02786
B	646	SER	-	expression tag	UNP P02786
B	647	HIS	-	expression tag	UNP P02786
B	648	HIS	-	expression tag	UNP P02786
B	649	HIS	-	expression tag	UNP P02786
B	650	HIS	-	expression tag	UNP P02786
B	651	HIS	-	expression tag	UNP P02786
B	652	HIS	-	expression tag	UNP P02786
B	653	GLY	-	expression tag	UNP P02786
B	654	GLY	-	expression tag	UNP P02786
B	655	GLY	-	expression tag	UNP P02786
B	656	SER	-	expression tag	UNP P02786
B	657	LEU	-	expression tag	UNP P02786
B	658	ASN	-	expression tag	UNP P02786
B	659	ASP	-	expression tag	UNP P02786
B	660	ILE	-	expression tag	UNP P02786
B	661	PHE	-	expression tag	UNP P02786
B	662	GLU	-	expression tag	UNP P02786
B	663	ALA	-	expression tag	UNP P02786
B	664	GLN	-	expression tag	UNP P02786
B	665	LYS	-	expression tag	UNP P02786
B	666	ILE	-	expression tag	UNP P02786
B	667	GLU	-	expression tag	UNP P02786
B	668	TRP	-	expression tag	UNP P02786
B	669	HIS	-	expression tag	UNP P02786
B	670	GLU	-	expression tag	UNP P02786

- Molecule 2 is a protein called transferrin receptor binding cystine-dense peptide.

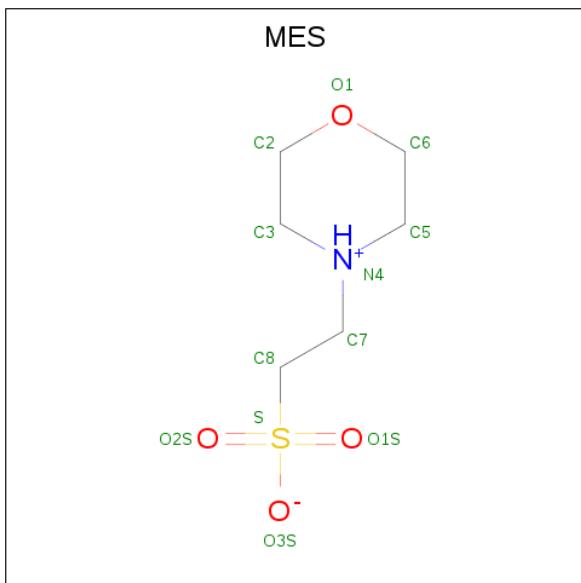
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	43	Total	C	N	O	S	0	0	0
			317	188	57	65	7			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	42	Total	C	N	O	S	0	1	0
			310	184	52	65	9			

- Molecule 3 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: $C_6H_{13}NO_4S$).



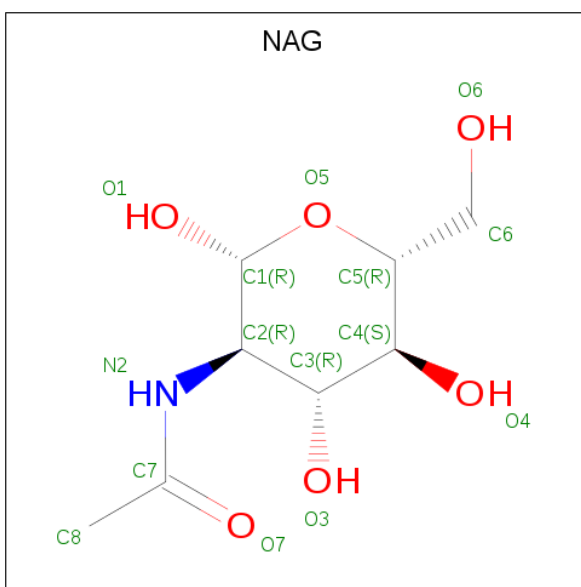
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
3	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- 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	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	B	1	Total	C	N	O	0	0
			14	8	1	5		
5	B	1	Total	C	N	O	0	0
			14	8	1	5		

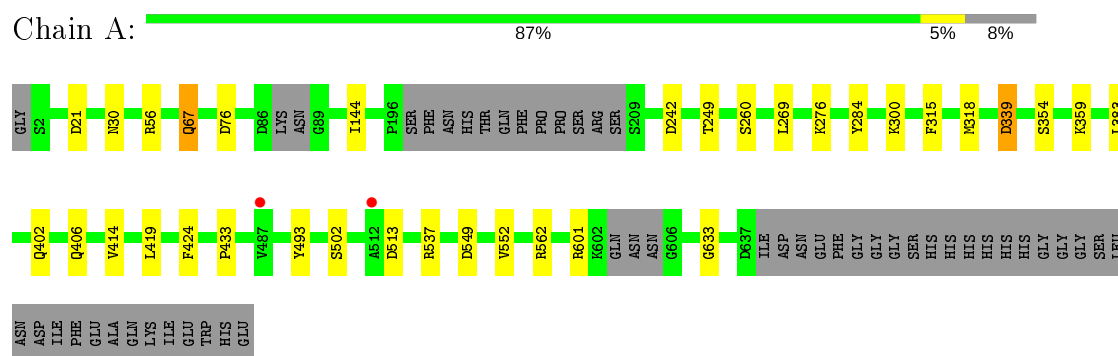
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	379	Total	O	0	0
			379	379		
6	B	366	Total	O	0	0
			366	366		
6	C	19	Total	O	0	0
			19	19		
6	D	18	Total	O	0	0
			18	18		

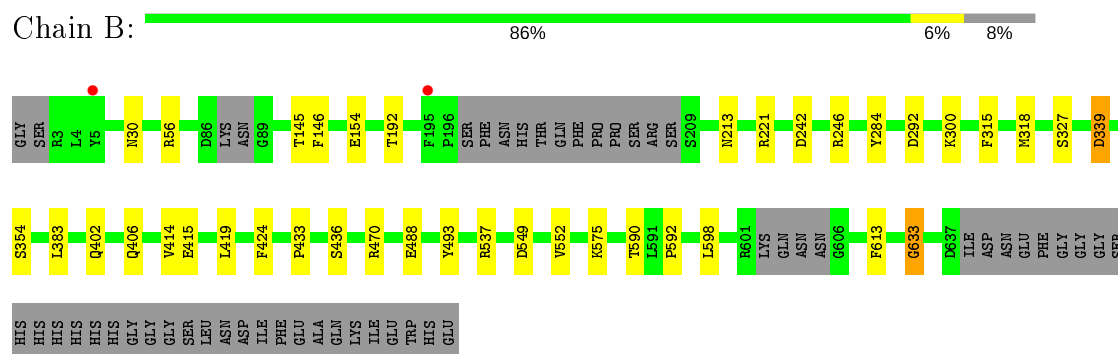
3 Residue-property plots [i](#)

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.

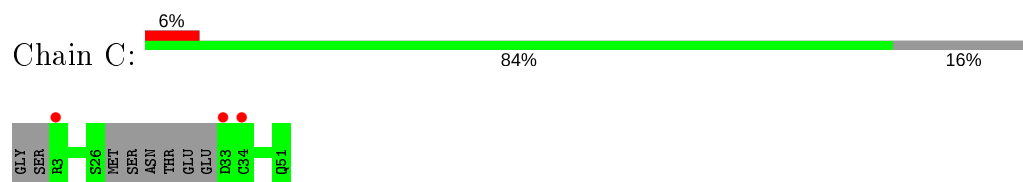
- Molecule 1: Transferrin receptor protein 1



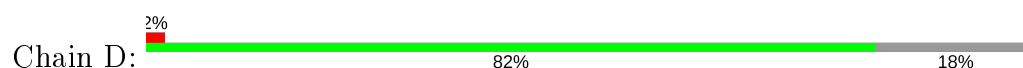
- Molecule 1: Transferrin receptor protein 1

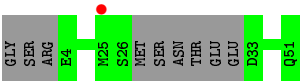


- Molecule 2: transferrin receptor binding cystine-dense peptide



- Molecule 2: transferrin receptor binding cystine-dense peptide





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	102.60Å 145.50Å 133.49Å 90.00° 90.02° 90.00°	Depositor
Resolution (Å)	50.01 – 1.85 49.18 – 1.85	Depositor EDS
% Data completeness (in resolution range)	99.4 (50.01-1.85) 99.4 (49.18-1.85)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.86 (at 1.84Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.163 , 0.187 0.174 , 0.196	Depositor DCC
R_{free} test set	8375 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	20.5	Xtriage
Anisotropy	0.299	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 23.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.479 for -h,-k,l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	11117	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.10% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, NAG, MES

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	0.82	0/4917	0.82	3/6685 (0.0%)
1	B	0.81	0/4901	0.82	6/6665 (0.1%)
2	C	0.64	0/319	0.66	0/427
2	D	0.72	0/315	0.72	0/422
All	All	0.81	0/10452	0.81	9/14199 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	5
1	B	0	5
All	All	0	10

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	B	537	ARG	NE-CZ-NH2	9.40	125.00	120.30
1	A	537	ARG	NE-CZ-NH1	9.24	124.92	120.30
1	B	537	ARG	NE-CZ-NH1	-7.72	116.44	120.30
1	A	537	ARG	NE-CZ-NH2	-7.21	116.70	120.30
1	A	56	ARG	NE-CZ-NH2	-5.52	117.54	120.30
1	B	292	ASP	CB-CG-OD2	5.34	123.11	118.30
1	B	56	ARG	NE-CZ-NH1	5.33	122.96	120.30
1	B	246	ARG	NE-CZ-NH1	5.28	122.94	120.30
1	B	56	ARG	NE-CZ-NH2	-5.02	117.79	120.30

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	21	ASP	Mainchain
1	A	242	ASP	Mainchain
1	A	354	SER	Mainchain
1	A	406	GLN	Mainchain
1	A	633	GLY	Mainchain
1	B	242	ASP	Mainchain
1	B	354	SER	Mainchain
1	B	406	GLN	Mainchain
1	B	575	LYS	Mainchain
1	B	633	GLY	Mainchain

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	4792	0	4647	23	0
1	B	4776	0	4635	30	0
2	C	317	0	259	0	0
2	D	310	0	252	0	0
3	A	12	0	13	0	0
3	B	12	0	13	0	0
4	A	24	0	32	7	0
4	B	36	0	48	5	0
5	A	28	0	26	0	0
5	B	28	0	26	0	0
6	A	379	0	0	5	0
6	B	366	0	0	4	0
6	C	19	0	0	0	0
6	D	18	0	0	0	0
All	All	11117	0	9951	53	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 3.

All (53) 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:B:192:THR:CB	6:B:833:HOH:O	2.04	1.03
1:B:414:VAL:CG1	6:B:973:HOH:O	2.25	0.84
1:A:144:ILE:HG21	4:A:705:GOL:H12	1.63	0.77
1:A:414:VAL:CG1	6:A:973:HOH:O	2.32	0.77
1:A:549:ASP:HB3	1:A:552:VAL:HG12	1.68	0.76
1:B:419:LEU:CD1	1:B:424:PHE:CE2	2.71	0.74
1:B:549:ASP:HB3	1:B:552:VAL:HG12	1.77	0.67
1:B:419:LEU:HD13	1:B:424:PHE:CE2	2.31	0.65
1:A:276:LYS:O	4:A:703:GOL:H31	1.97	0.65
1:B:146:PHE:H	4:B:706:GOL:C1	2.14	0.60
1:B:315:PHE:CD1	1:B:318:MET:CE	2.85	0.59
1:A:419:LEU:CD1	1:A:424:PHE:CE2	2.87	0.58
1:B:415:GLU:HA	4:B:707:GOL:H31	1.86	0.58
1:B:315:PHE:CD1	1:B:318:MET:HE3	2.39	0.57
1:B:436:SER:OG	4:B:702:GOL:H12	2.03	0.57
1:B:470:ARG:HH11	1:B:470:ARG:HG2	1.69	0.57
1:A:549:ASP:HB3	1:A:552:VAL:CG1	2.35	0.56
1:A:562:ARG:HD2	6:A:1063:HOH:O	2.07	0.54
1:A:276:LYS:HB2	4:A:703:GOL:C3	2.38	0.54
1:A:414:VAL:HG12	6:A:973:HOH:O	2.03	0.52
1:B:315:PHE:CE1	1:B:318:MET:HE1	2.44	0.51
1:A:315:PHE:HA	1:A:318:MET:HE3	1.93	0.51
1:A:276:LYS:HB2	4:A:703:GOL:H32	1.92	0.51
4:A:703:GOL:H32	6:A:906:HOH:O	2.11	0.51
1:B:383:LEU:HD12	1:B:433:PRO:HG3	1.93	0.50
1:A:300:LYS:HD3	1:A:339:ASP:OD1	2.12	0.49
1:B:146:PHE:H	4:B:706:GOL:H11	1.77	0.49
1:B:300:LYS:HD3	1:B:339:ASP:OD1	2.12	0.49
1:B:383:LEU:HD22	1:B:493:TYR:HA	1.94	0.49
1:B:383:LEU:CD2	1:B:493:TYR:HA	2.42	0.49
1:A:419:LEU:HD12	1:A:424:PHE:CE2	2.47	0.48
1:B:470:ARG:HG2	1:B:470:ARG:NH1	2.29	0.48
1:B:315:PHE:HA	1:B:318:MET:HE2	1.96	0.48
1:B:154:GLU:OE2	1:B:213:ASN:HB2	2.15	0.47
1:B:549:ASP:HB3	1:B:552:VAL:CG1	2.44	0.47
1:B:419:LEU:HD12	1:B:424:PHE:CD2	2.49	0.47
1:A:383:LEU:HD12	1:A:433:PRO:HG3	1.97	0.46
1:A:383:LEU:HD22	1:A:493:TYR:HA	1.98	0.46
1:A:144:ILE:CG2	4:A:705:GOL:H12	2.40	0.46
1:A:67:GLN:HB2	1:A:269:LEU:HD23	1.98	0.45
1:A:402:GLN:NE2	6:A:805:HOH:O	2.32	0.45
1:B:598:LEU:HD22	1:B:613:PHE:CE1	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:549:ASP:O	1:A:552:VAL:HG12	2.18	0.44
1:B:402:GLN:NE2	6:B:805:HOH:O	2.33	0.43
1:B:315:PHE:CE1	1:B:318:MET:CE	3.02	0.42
1:A:513:ASP:OD2	1:A:601:ARG:NH1	2.51	0.42
1:B:590:THR:HB	1:B:592:PRO:HD2	2.00	0.42
1:A:76:ASP:HB2	1:A:260:SER:O	2.19	0.42
1:B:414:VAL:HG12	6:B:973:HOH:O	2.03	0.41
1:A:276:LYS:HB2	4:A:703:GOL:H31	2.03	0.40
1:A:359:LYS:HE2	1:B:633:GLY:O	2.21	0.40
1:B:145:THR:HB	4:B:706:GOL:H12	2.04	0.40
1:B:221:ARG:HD3	1:B:221:ARG:HH11	1.65	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	616/670 (92%)	598 (97%)	18 (3%)	0	100	100
1	B	614/670 (92%)	597 (97%)	17 (3%)	0	100	100
2	C	39/51 (76%)	38 (97%)	1 (3%)	0	100	100
2	D	39/51 (76%)	37 (95%)	2 (5%)	0	100	100
All	All	1308/1442 (91%)	1270 (97%)	38 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	504/571 (88%)	498 (99%)	6 (1%)	71	62
1	B	501/571 (88%)	496 (99%)	5 (1%)	76	69
2	C	32/47 (68%)	32 (100%)	0	100	100
2	D	33/47 (70%)	33 (100%)	0	100	100
All	All	1070/1236 (87%)	1059 (99%)	11 (1%)	76	69

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	ASN
1	A	67	GLN
1	A	249	THR
1	A	284	TYR
1	A	339	ASP
1	A	502	SER
1	B	30	ASN
1	B	284	TYR
1	B	327	SER
1	B	339	ASP
1	B	488	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	152	ASN
1	A	365	ASN
1	B	509	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 [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

16 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	A	707	1	14,14,15	0.46	0	17,19,21	0.61	0
4	GOL	A	705	-	5,5,5	0.62	0	5,5,5	0.74	0
5	NAG	A	706	1	14,14,15	0.50	0	17,19,21	1.03	1 (5%)
4	GOL	B	702	-	5,5,5	0.24	0	5,5,5	1.01	1 (20%)
4	GOL	B	705	-	5,5,5	0.60	0	5,5,5	0.75	0
4	GOL	B	706	-	5,5,5	0.57	0	5,5,5	1.93	1 (20%)
3	MES	A	701	-	12,12,12	1.73	1 (8%)	14,16,16	0.98	1 (7%)
4	GOL	A	704	-	5,5,5	0.59	0	5,5,5	0.75	0
4	GOL	A	703	-	5,5,5	0.25	0	5,5,5	0.58	0
4	GOL	B	703	-	5,5,5	0.42	0	5,5,5	0.69	0
5	NAG	B	708	1	14,14,15	0.40	0	17,19,21	0.90	1 (5%)
4	GOL	B	707	-	5,5,5	0.25	0	5,5,5	0.95	0
5	NAG	B	709	1	14,14,15	0.49	0	17,19,21	0.62	0
3	MES	B	701	-	12,12,12	1.63	1 (8%)	14,16,16	1.06	0
4	GOL	A	702	-	5,5,5	0.52	0	5,5,5	1.07	0
4	GOL	B	704	-	5,5,5	0.63	0	5,5,5	0.39	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
5	NAG	A	707	1	-	0/6/23/26	0/1/1/1
4	GOL	A	705	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	A	706	1	-	0/6/23/26	0/1/1/1
4	GOL	B	702	-	-	0/4/4/4	-
4	GOL	B	705	-	-	4/4/4/4	-
4	GOL	B	706	-	-	3/4/4/4	-
3	MES	A	701	-	-	1/6/14/14	0/1/1/1
4	GOL	A	704	-	-	4/4/4/4	-
4	GOL	A	703	-	-	2/4/4/4	-
4	GOL	B	703	-	-	2/4/4/4	-
5	NAG	B	708	1	-	0/6/23/26	0/1/1/1
4	GOL	B	707	-	-	2/4/4/4	-
5	NAG	B	709	1	-	0/6/23/26	0/1/1/1
3	MES	B	701	-	-	0/6/14/14	0/1/1/1
4	GOL	A	702	-	-	0/4/4/4	-
4	GOL	B	704	-	-	2/4/4/4	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	701	MES	C8-S	-5.67	1.69	1.77
3	B	701	MES	C8-S	-5.29	1.70	1.77

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	706	GOL	C3-C2-C1	-3.81	96.89	111.70
3	A	701	MES	C5-N4-C3	2.48	114.42	108.83
5	A	706	NAG	O5-C5-C6	2.20	110.65	107.20
4	B	702	GOL	C3-C2-C1	-2.16	103.31	111.70
5	B	708	NAG	O3-C3-C2	-2.02	105.29	109.47

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	705	GOL	C1-C2-C3-O3
4	B	706	GOL	C1-C2-C3-O3
4	A	704	GOL	C1-C2-C3-O3
4	B	707	GOL	O1-C1-C2-C3
4	B	705	GOL	O2-C2-C3-O3
4	B	707	GOL	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
4	A	705	GOL	C1-C2-C3-O3
4	B	705	GOL	O1-C1-C2-C3
4	A	704	GOL	O1-C1-C2-C3
4	A	703	GOL	C1-C2-C3-O3
4	B	703	GOL	O1-C1-C2-C3
4	B	704	GOL	O1-C1-C2-C3
4	A	704	GOL	O2-C2-C3-O3
4	B	706	GOL	O2-C2-C3-O3
4	A	705	GOL	O2-C2-C3-O3
4	B	705	GOL	O1-C1-C2-O2
4	A	703	GOL	O2-C2-C3-O3
4	A	704	GOL	O1-C1-C2-O2
4	B	703	GOL	O1-C1-C2-O2
4	B	704	GOL	O1-C1-C2-O2
3	A	701	MES	C8-C7-N4-C3
4	B	706	GOL	O1-C1-C2-C3

There are no ring outliers.

5 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	705	GOL	2	0
4	B	702	GOL	1	0
4	B	706	GOL	3	0
4	A	703	GOL	5	0
4	B	707	GOL	1	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 [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	619/670 (92%)	-0.40	2 (0%) 94 93	12, 23, 50, 84	0
1	B	617/670 (92%)	-0.42	2 (0%) 94 93	12, 23, 49, 73	0
2	C	43/51 (84%)	0.24	3 (6%) 16 15	24, 36, 65, 79	0
2	D	42/51 (82%)	-0.06	1 (2%) 59 57	24, 36, 66, 83	0
All	All	1321/1442 (91%)	-0.38	8 (0%) 89 89	12, 24, 52, 84	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	195	PHE	2.9
2	C	3	ARG	2.8
2	C	34	CYS	2.8
1	B	5	TYR	2.8
1	A	487	VAL	2.7
2	C	33	ASP	2.7
1	A	512	ALA	2.6
2	D	25	MET	2.1

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

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
4	GOL	A	704	6/6	0.78	0.17	38,47,52,53	0
4	GOL	B	705	6/6	0.79	0.17	37,44,48,50	0
4	GOL	A	703	6/6	0.80	0.21	37,51,55,56	0
4	GOL	B	704	6/6	0.82	0.23	38,45,53,65	0
4	GOL	A	702	6/6	0.85	0.14	33,42,49,49	0
5	NAG	A	707	14/15	0.86	0.23	43,51,59,61	0
4	GOL	A	705	6/6	0.88	0.24	31,42,48,74	0
5	NAG	A	706	14/15	0.89	0.17	24,35,50,51	0
5	NAG	B	709	14/15	0.90	0.18	42,50,60,62	0
4	GOL	B	702	6/6	0.90	0.13	23,33,42,67	0
4	GOL	B	707	6/6	0.90	0.22	26,46,49,55	0
4	GOL	B	703	6/6	0.91	0.18	35,49,57,60	0
5	NAG	B	708	14/15	0.92	0.11	25,37,52,54	0
4	GOL	B	706	6/6	0.93	0.16	19,31,41,45	0
3	MES	B	701	12/12	0.98	0.08	18,20,21,22	0
3	MES	A	701	12/12	0.99	0.07	17,19,21,22	0

6.5 Other polymers

There are no such residues in this entry.