W O R L D W I D E

wwPDB

P R O T E I N   D A T A   B A N K

Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 05:02 PM GMT

PDB ID	:	4GXG
Title	:	Crystal structure of human GLTP bound with 12:0 monosulfatide (orthorhombic form; four subunits in asymmetric unit)
Authors	:	Samygina, V.R.; Cabo-Bilbao, A.; Goni-de-Cerio, F.; Popov, A.N.; Malinina, L.
Deposited on	:	2012-09-04
Resolution	:	2.40 Å(reported)

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

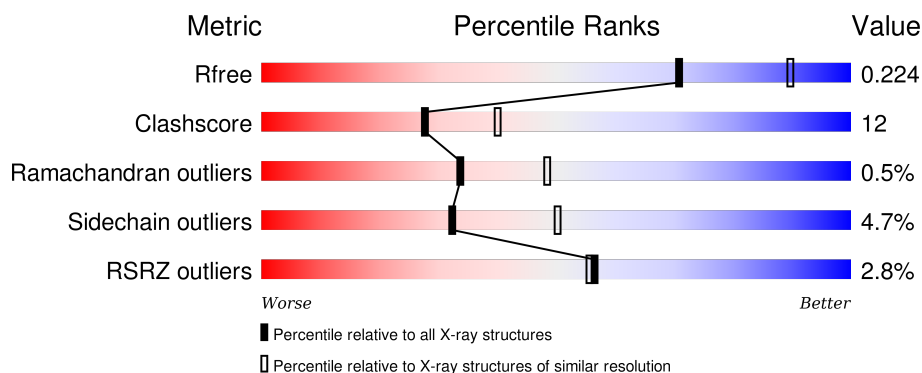|		
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 2.40 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	Percentile Ranks	Value
Rfree		0.224
Clashscore		12
Ramachandran outliers		0.5%
Sidechain outliers		4.7%
RSRZ outliers		2.8%

Worse   *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	91344	2919 (2.40-2.40)
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (2.40-2.40)

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. 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.

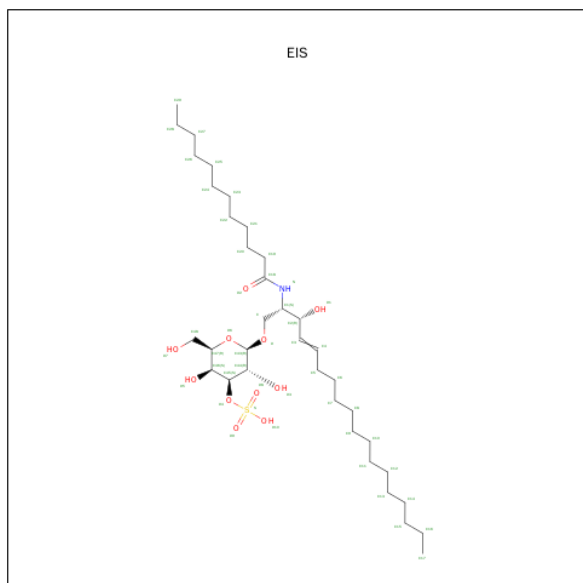| Mol	Chain	Length	Quality of chain
1	A	209	2% 80% 16% •
1	B	209	3% 83% 15% ••
1	D	209	4% 78% 18% •••
1	E	209	2% 80% 16% •

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 7167 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 Glycolipid transfer protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	209	Total 1693	C 1102	N 275	O 306	S 10	0	3	0
1	B	207	Total 1680	C 1094	N 273	O 304	S 9	0	3	0
1	D	206	Total 1672	C 1088	N 272	O 303	S 9	0	3	0
1	E	208	Total 1685	C 1097	N 274	O 305	S 9	0	3	0

- Molecule 2 is N-{(2S,3R,4E)-3-HYDROXY-1-[(3-O-SULFO-BETA-D-GALACTOPYRAN OSYL)OXY]OCTADEC-4-EN-2-YL}DODECANAMIDE (three-letter code: EIS) (formula: $C_{36}H_{69}NO_{11}S$).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 49	C 36	N 1	O 11	S 1	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	N	O	S	0	0
			49	36	1	11	1		
2	D	1	Total	C	N	O	S	0	0
			49	36	1	11	1		
2	E	1	Total	C	N	O	S	0	0
			45	32	1	11	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	82	Total	O	0	0
			82	82		
3	B	54	Total	O	0	0
			54	54		
3	D	45	Total	O	0	0
			45	45		
3	E	64	Total	O	0	0
			64	64		

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded accord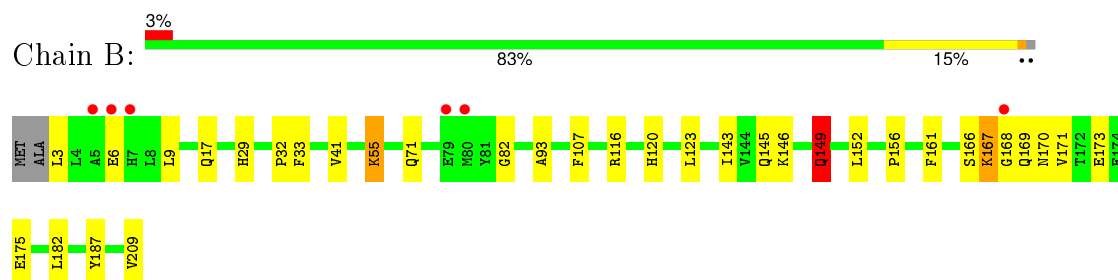ing to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.
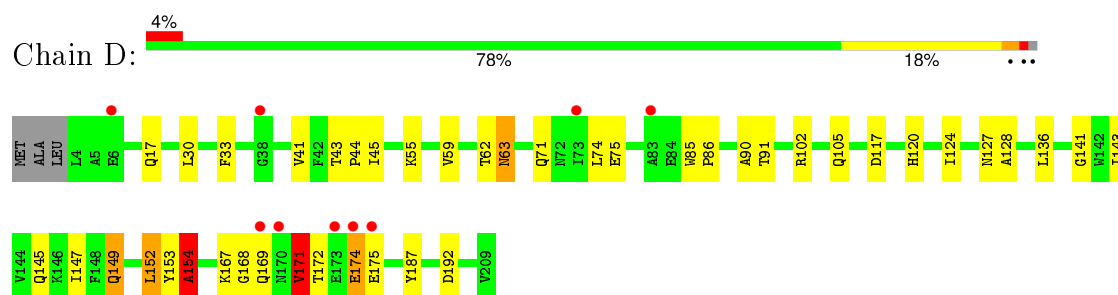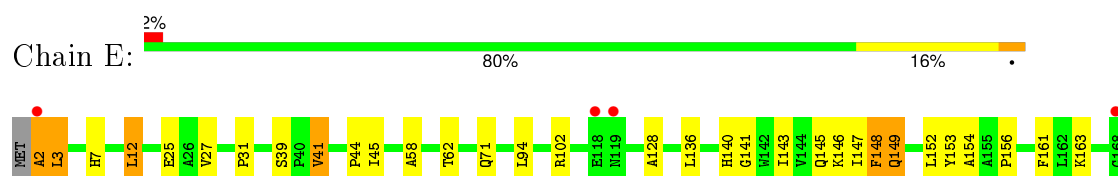
- Molecule 1: Glycolipid transfer protein

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- Molecule 1: Glycolipid transfer protein

Q169 N170 V171 T172 E173 E174 E175 E178 D192 V193 Y198 V209

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	65.20Å 84.65Å 171.88Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	14.98 – 2.40 14.97 – 2.40	Depositor EDS
% Data completeness (in resolution range)	97.8 (14.98-2.40) 97.8 (14.97-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.70 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.207 , 0.271 0.210 , 0.224	Depositor DCC
R_{free} test set	1884 reflections (5.36%)	DCC
Wilson B-factor (Å^2)	34.6	Xtriage
Anisotropy	0.030	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 36.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< |L| > = 0.48, < L^2 > = 0.31$	Xtriage
Outliers	0 of 37037 reflections	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	7167	wwPDB-VP
Average B, all atoms (Å^2)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.07% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: EIS

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	0.73	2/1747 (0.1%)	0.71	0/2365
1	B	0.64	0/1734	0.72	2/2348 (0.1%)
1	D	0.66	2/1726 (0.1%)	0.65	2/2337 (0.1%)
1	E	0.79	2/1739 (0.1%)	0.73	2/2355 (0.1%)
All	All	0.71	6/6946 (0.1%)	0.70	6/9405 (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	D	0	4
1	E	0	1
All	All	0	5

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	174[A]	GLU	CB-CG	13.21	1.77	1.52
1	E	174[B]	GLU	CB-CG	13.21	1.77	1.52
1	A	174[A]	GLU	CB-CG	7.87	1.67	1.52
1	A	174[B]	GLU	CB-CG	7.87	1.67	1.52
1	D	174[A]	GLU	CB-CG	7.54	1.66	1.52
1	D	174[B]	GLU	CB-CG	7.54	1.66	1.52

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	174[A]	GLU	CA-CB-CG	-6.30	99.55	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	174[B]	GLU	CA-CB-CG	-6.30	99.55	113.40
1	D	149[A]	GLN	N-CA-CB	5.12	119.81	110.60
1	D	149[B]	GLN	N-CA-CB	5.12	119.81	110.60
1	B	149[A]	GLN	N-CA-CB	5.05	119.69	110.60
1	B	149[B]	GLN	N-CA-CB	5.05	119.69	110.60

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	154	ALA	Peptide
1	D	167	LYS	Peptide
1	D	168	GLY	Peptide
1	D	171	VAL	Peptide
1	E	2	ALA	Peptide

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	1693	0	1721	44	0
1	B	1680	0	1704	25	0
1	D	1672	0	1693	56	0
1	E	1685	0	1709	35	0
2	A	49	0	67	5	0
2	B	49	0	67	5	0
2	D	49	0	67	15	0
2	E	45	0	56	16	0
3	A	82	0	0	5	0
3	B	54	0	0	4	0
3	D	45	0	0	0	0
3	E	64	0	0	3	0
All	All	7167	0	7084	165	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 12.

All (165) 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:D:171:VAL:HG22	1:D:172:THR:HG23	1.20	1.11
1:A:154:ALA:HB2	1:B:143:ILE:HD13	1.45	0.98
2:D:700:EIS:H43	1:E:148:PHE:CE1	2.00	0.97
1:E:136:LEU:CD1	2:E:700:EIS:H59	1.94	0.97
1:B:166:SER:O	1:B:167:LYS:HG3	1.64	0.96
1:D:172:THR:OG1	1:D:175:GLU:HB3	1.66	0.94
1:D:171:VAL:CG2	1:D:172:THR:HG23	1.97	0.94
1:D:171:VAL:CG1	1:D:175:GLU:HG2	1.99	0.93
1:B:149[A]:GLN:HG2	3:B:825:HOH:O	1.68	0.92
1:D:171:VAL:HG12	1:D:175:GLU:HG2	1.54	0.89
1:D:171:VAL:HG12	1:D:175:GLU:CG	2.03	0.88
1:D:172:THR:OG1	1:D:175:GLU:CB	2.22	0.87
1:B:166:SER:C	1:B:167:LYS:HG3	1.93	0.85
1:E:45:ILE:HG23	2:E:700:EIS:C22	2.10	0.82
3:A:805:HOH:O	1:D:120:HIS:HE1	1.61	0.82
1:E:136:LEU:HD11	2:E:700:EIS:H59	1.61	0.81
1:D:171:VAL:HG13	1:D:172:THR:OG1	1.81	0.80
1:D:171:VAL:CG1	1:D:175:GLU:HB3	2.12	0.79
1:E:2:ALA:HA	1:E:3:LEU:C	2.02	0.79
1:D:30:LEU:O	1:D:33:PHE:HB3	1.81	0.79
1:D:171:VAL:HG22	1:D:172:THR:CG2	2.07	0.78
2:D:700:EIS:C17	2:E:700:EIS:H21	2.13	0.78
1:B:120:HIS:HB3	1:B:123:LEU:HD12	1.64	0.78
1:A:145:GLN:O	1:A:149[B]:GLN:HG3	1.84	0.77
1:E:45:ILE:HG23	2:E:700:EIS:H63	1.67	0.77
1:D:153:TYR:O	1:D:154:ALA:CB	2.31	0.77
1:A:3:LEU:CD2	1:A:167:LYS:NZ	2.48	0.76
1:A:142:TRP:CZ3	1:A:146:LYS:HE3	2.22	0.74
1:D:62:THR:O	1:D:63:ASN:HB2	1.87	0.74
1:D:171:VAL:CG1	1:D:175:GLU:CG	2.65	0.74
1:E:153:TYR:O	1:E:154:ALA:HB3	1.87	0.73
1:D:171:VAL:CG1	1:D:175:GLU:CB	2.66	0.73
1:A:167:LYS:CE	1:A:168:GLY:H	2.00	0.73
1:E:7:HIS:NE2	1:E:25:GLU:OE1	2.21	0.73
2:D:700:EIS:H44	2:E:700:EIS:H21	1.71	0.72
1:D:171:VAL:HG13	1:D:175:GLU:HB3	1.70	0.71
1:B:146:LYS:HG2	3:B:853:HOH:O	1.91	0.71
1:A:3:LEU:HD22	1:A:167:LYS:HZ1	1.56	0.70
1:A:167:LYS:N	1:A:167:LYS:HE2	2.05	0.70
2:A:700:EIS:H30	2:B:700:EIS:H33	1.72	0.70
1:B:145:GLN:O	1:B:149[B]:GLN:HG3	1.90	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:167:LYS:CD	1:A:168:GLY:H	2.04	0.70
1:E:178:GLU:HB2	3:E:836:HOH:O	1.90	0.70
1:E:136:LEU:HD13	2:E:700:EIS:H59	1.73	0.69
1:D:172:THR:HG1	1:D:175:GLU:HB3	1.57	0.67
1:D:45:ILE:HG23	2:D:700:EIS:H63	1.76	0.67
2:D:700:EIS:C16	2:E:700:EIS:H21	2.25	0.67
1:A:41:VAL:O	2:B:700:EIS:H35	1.95	0.67
2:D:700:EIS:H46	2:E:700:EIS:C5	2.25	0.66
1:A:167:LYS:HD2	1:A:168:GLY:H	1.60	0.65
1:B:169:GLN:HG3	3:B:833:HOH:O	1.94	0.65
1:B:171:VAL:HG22	1:B:175:GLU:HB2	1.78	0.65
1:D:171:VAL:HG11	1:D:175:GLU:HG2	1.79	0.65
1:A:3:LEU:HD23	1:A:3:LEU:N	2.11	0.65
1:B:171:VAL:HG22	1:B:175:GLU:CB	2.27	0.64
2:D:700:EIS:H44	2:E:700:EIS:H26	1.78	0.64
1:D:145:GLN:O	1:D:149[B]:GLN:HG3	1.99	0.63
1:A:3:LEU:CD2	1:A:167:LYS:HZ2	2.12	0.63
1:D:102:ARG:NH2	1:D:192:ASP:OD1	2.31	0.62
1:D:171:VAL:HG12	1:D:175:GLU:CB	2.29	0.62
1:A:166:SER:C	1:A:167:LYS:HE2	2.20	0.62
1:E:39:SER:OG	1:E:41:VAL:HG13	2.01	0.61
2:D:700:EIS:H31	1:E:44:PRO:HG2	1.81	0.61
1:E:12:LEU:HD22	1:E:193:VAL:HG21	1.82	0.61
1:D:171:VAL:HG12	1:D:175:GLU:HB3	1.82	0.60
1:D:74:LEU:HG	1:D:91:THR:HG23	1.84	0.60
1:B:120:HIS:CB	1:B:123:LEU:HD12	2.33	0.59
1:A:3:LEU:HD22	1:A:167:LYS:NZ	2.15	0.59
1:B:167:LYS:CD	1:B:168:GLY:H	2.14	0.59
1:D:45:ILE:CG2	2:D:700:EIS:H63	2.33	0.59
1:D:136:LEU:HD11	2:D:700:EIS:H66	1.85	0.58
1:E:141:GLY:O	1:E:145:GLN:HG3	2.03	0.58
1:D:171:VAL:HG13	1:D:172:THR:CG2	2.34	0.58
1:D:154:ALA:HB2	1:E:143:ILE:HD13	1.85	0.58
1:A:166:SER:HB3	1:A:171:VAL:HG12	1.86	0.57
2:D:700:EIS:H46	2:E:700:EIS:H22	1.86	0.57
1:A:166:SER:O	1:A:167:LYS:C	2.42	0.57
1:D:153:TYR:O	1:D:154:ALA:HB3	2.05	0.56
1:B:55:LYS:HD2	1:B:93:ALA:HB2	1.87	0.56
1:D:153:TYR:O	1:D:154:ALA:HB2	2.03	0.56
1:A:3:LEU:CD2	1:A:167:LYS:HZ1	2.16	0.56
1:D:85:TRP:CG	1:D:86:PRO:HA	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:147:ILE:HD13	2:A:700:EIS:H32	1.87	0.55
1:A:2:ALA:O	1:A:3:LEU:HB2	2.06	0.55
2:D:700:EIS:C17	2:E:700:EIS:C5	2.82	0.54
1:D:117:ASP:OD2	1:D:120:HIS:HD2	1.89	0.54
1:D:172:THR:OG1	1:D:175:GLU:HB2	2.07	0.53
1:E:156:PRO:HG2	1:E:161:PHE:HB2	1.90	0.53
1:D:171:VAL:HG13	1:D:175:GLU:CB	2.37	0.53
1:D:128:ALA:CB	1:D:152:LEU:HD21	2.39	0.53
1:A:151:ALA:O	1:A:153:TYR:O	2.27	0.53
1:E:175:GLU:O	1:E:178:GLU:HG2	2.08	0.53
1:D:171:VAL:HG13	1:D:172:THR:HG23	1.91	0.52
1:A:143:ILE:HG12	3:A:859:HOH:O	2.09	0.52
1:E:102:ARG:HD2	3:E:858:HOH:O	2.10	0.52
2:D:700:EIS:H43	1:E:148:PHE:HE1	1.68	0.52
1:B:116:ARG:HD3	3:B:818:HOH:O	2.09	0.52
1:A:124:ILE:HD11	1:A:156:PRO:HD2	1.93	0.51
1:E:94:LEU:HB3	1:E:198:TYR:OH	2.10	0.51
1:A:167:LYS:HE3	1:A:168:GLY:H	1.73	0.51
1:D:171:VAL:O	1:D:175:GLU:HB3	2.11	0.50
1:A:136:LEU:HD13	2:A:700:EIS:H64	1.93	0.50
1:D:43:THR:HB	1:D:44:PRO:HD3	1.93	0.50
1:A:45:ILE:HD13	2:A:700:EIS:H56	1.94	0.50
1:B:167:LYS:HD2	1:B:168:GLY:H	1.77	0.49
1:A:71:GLN:NE2	1:A:201:MET:SD	2.85	0.49
1:E:128:ALA:HB1	1:E:152:LEU:HD22	1.94	0.48
1:E:2:ALA:CA	1:E:3:LEU:C	2.76	0.48
1:E:146:LYS:HA	1:E:149[B]:GLN:HG2	1.94	0.48
1:E:2:ALA:HA	1:E:3:LEU:O	2.14	0.48
1:A:44:PRO:HG2	2:B:700:EIS:H29	1.96	0.48
1:A:156:PRO:HG2	1:A:161:PHE:HB2	1.96	0.48
1:E:27:VAL:O	1:E:31:PRO:HD3	2.15	0.47
1:B:3:LEU:HD12	1:B:6:GLU:OE2	2.15	0.47
1:E:102:ARG:NH2	1:E:192:ASP:OD1	2.48	0.46
1:D:171:VAL:CG1	1:D:172:THR:HG23	2.46	0.46
1:E:140:HIS:NE2	2:E:700:EIS:O2	2.41	0.46
1:D:128:ALA:HB3	1:D:152:LEU:HD21	1.96	0.46
1:A:24:LEU:HA	1:A:27:VAL:HG22	1.97	0.46
1:A:167:LYS:CE	1:A:168:GLY:N	2.75	0.46
1:A:3:LEU:CD2	1:A:3:LEU:N	2.78	0.46
1:B:171:VAL:HG22	1:B:175:GLU:HB3	1.96	0.46
1:A:120:HIS:HE1	3:A:862:HOH:O	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:805:HOH:O	1:D:120:HIS:CE1	2.47	0.46
1:D:147:ILE:HG23	1:E:147:ILE:HG23	1.98	0.46
1:A:153:TYR:O	1:A:154:ALA:HB3	2.15	0.45
2:D:700:EIS:H27	1:E:41:VAL:HA	1.99	0.45
1:B:170:ASN:N	1:B:170:ASN:OD1	2.47	0.45
1:A:172:THR:OG1	1:A:175:GLU:HG3	2.16	0.45
1:D:30:LEU:O	1:D:33:PHE:CB	2.60	0.45
1:B:166:SER:O	1:B:167:LYS:CG	2.50	0.45
1:D:105:GLN:HB2	1:D:187:TYR:CE2	2.51	0.45
1:A:154:ALA:CB	1:B:143:ILE:HD13	2.32	0.44
2:D:700:EIS:H45	2:E:700:EIS:H67	1.98	0.44
1:D:71:GLN:HE21	1:D:75:GLU:HG3	1.81	0.44
1:E:58:ALA:O	1:E:62:THR:HG23	2.18	0.44
1:A:187:TYR:CZ	1:A:191:ILE:HD11	2.53	0.44
1:D:171:VAL:HG13	1:D:172:THR:CB	2.47	0.44
1:B:33:PHE:HZ	1:B:107:PHE:CD2	2.36	0.44
1:A:77:GLU:O	1:A:81:TYR:HD2	2.01	0.43
1:B:29:HIS:O	1:B:32:PRO:HD2	2.18	0.43
1:B:17:GLN:HE22	1:B:71:GLN:HB3	1.84	0.43
1:B:156:PRO:HG2	1:B:161:PHE:HB2	2.01	0.42
1:A:125:ARG:HD3	3:A:856:HOH:O	2.19	0.42
1:D:45:ILE:HG12	2:E:700:EIS:H39	2.02	0.42
1:A:147:ILE:HG22	2:B:700:EIS:H40	2.02	0.42
1:D:141:GLY:O	1:D:145:GLN:HG3	2.19	0.42
1:D:117:ASP:OD2	1:D:120:HIS:CD2	2.72	0.42
1:E:2:ALA:CA	1:E:3:LEU:O	2.67	0.42
1:B:9:LEU:HD22	1:B:187:TYR:HA	2.02	0.42
1:D:124:ILE:HA	1:D:127:ASN:HD22	1.84	0.42
1:A:44:PRO:HG2	2:B:700:EIS:H34	2.01	0.42
1:D:55:LYS:O	1:D:59:VAL:HG23	2.20	0.42
1:D:59:VAL:HG21	1:D:90:ALA:HB2	2.02	0.41
1:A:39:SER:HA	1:A:40:PRO:HD2	1.82	0.41
1:E:163:LYS:HD2	3:E:850:HOH:O	2.20	0.41
1:A:3:LEU:HD21	1:A:167:LYS:NZ	2.31	0.41
1:D:17:GLN:HE22	1:D:71:GLN:HB3	1.86	0.41
1:A:185:VAL:HG12	1:A:186:ASN:N	2.36	0.41
1:A:147:ILE:CD1	2:A:700:EIS:H32	2.50	0.40
1:D:41:VAL:HA	2:E:700:EIS:H28	2.02	0.40
1:D:17:GLN:HE22	1:D:71:GLN:CB	2.35	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	210/209 (100%)	202 (96%)	7 (3%)	1 (0%)	34	48
1	B	208/209 (100%)	197 (95%)	10 (5%)	1 (0%)	34	48
1	D	207/209 (99%)	193 (93%)	12 (6%)	2 (1%)	19	28
1	E	209/209 (100%)	198 (95%)	11 (5%)	0	100	100
All	All	834/836 (100%)	790 (95%)	40 (5%)	4 (0%)	34	48

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	167	LYS
1	D	63	ASN
1	D	154	ALA
1	B	82	GLY

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	183/180 (102%)	170 (93%)	13 (7%)	18	28
1	B	182/180 (101%)	173 (95%)	9 (5%)	31	48
1	D	181/180 (101%)	175 (97%)	6 (3%)	45	66
1	E	182/180 (101%)	170 (93%)	12 (7%)	21	32
All	All	728/720 (101%)	688 (94%)	40 (6%)	32	42

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	LEU
1	A	33	PHE
1	A	41	VAL
1	A	49	ILE
1	A	142	TRP
1	A	149[A]	GLN
1	A	149[B]	GLN
1	A	152	LEU
1	A	167	LYS
1	A	171	VAL
1	A	172	THR
1	A	174[A]	GLU
1	A	174[B]	GLU
1	B	41	VAL
1	B	55	LYS
1	B	149[A]	GLN
1	B	149[B]	GLN
1	B	152	LEU
1	B	167	LYS
1	B	173	GLU
1	B	182	LEU
1	B	209	VAL
1	D	143	ILE
1	D	152	LEU
1	D	169	GLN
1	D	171	VAL
1	D	174[A]	GLU
1	D	174[B]	GLU
1	E	3	LEU
1	E	12	LEU
1	E	41	VAL
1	E	71	GLN
1	E	148	PHE
1	E	149[A]	GLN
1	E	149[B]	GLN
1	E	170	ASN
1	E	171	VAL
1	E	173	GLU
1	E	174[A]	GLU
1	E	174[B]	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	7	HIS
1	A	17	GLN
1	A	120	HIS
1	A	127	ASN
1	A	206	ASN
1	B	17	GLN
1	B	29	HIS
1	B	127	ASN
1	B	169	GLN
1	D	17	GLN
1	D	120	HIS
1	D	127	ASN
1	D	169	GLN
1	E	29	HIS
1	E	71	GLN
1	E	127	ASN
1	E	169	GLN
1	E	170	ASN
1	E	206	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 carbohydrates in this entry.

5.6 Ligand geometry (i)

4 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	#$|Z| > 2$
2	EIS	A	700	-	48,49,49	2.08	6 (12%)	54,60,60	2.88	11 (20%)
2	EIS	B	700	-	48,49,49	2.14	6 (12%)	54,60,60	4.98	8 (14%)
2	EIS	D	700	-	48,49,49	2.01	6 (12%)	54,60,60	5.04	8 (14%)
2	EIS	E	700	-	44,45,49	2.17	6 (13%)	50,56,60	2.79	8 (16%)

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
2	EIS	A	700	-	-	0/46/66/66	0/1/1/1
2	EIS	B	700	-	-	1/46/66/66	0/1/1/1
2	EIS	D	700	-	-	0/46/66/66	0/1/1/1
2	EIS	E	700	-	-	0/42/62/66	0/1/1/1

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	700	EIS	O4-C45	-6.51	1.32	1.46
2	A	700	EIS	O-C	-5.95	1.32	1.43
2	B	700	EIS	O-C	-5.92	1.32	1.43
2	E	700	EIS	O4-C45	-5.85	1.34	1.46
2	D	700	EIS	O4-C45	-5.73	1.34	1.46
2	D	700	EIS	O-C	-5.68	1.33	1.43
2	E	700	EIS	O-C	-5.50	1.33	1.43
2	A	700	EIS	O4-C45	-5.45	1.34	1.46
2	A	700	EIS	C18-N	-4.19	1.25	1.34
2	B	700	EIS	C18-N	-3.94	1.26	1.34
2	E	700	EIS	C18-N	-3.93	1.26	1.34
2	D	700	EIS	C18-N	-3.20	1.27	1.34
2	B	700	EIS	O4-S	-3.14	1.47	1.57
2	D	700	EIS	O4-S	-3.10	1.47	1.57
2	E	700	EIS	O4-S	-3.04	1.47	1.57
2	A	700	EIS	O4-S	-2.92	1.47	1.57
2	D	700	EIS	C3-C4	3.31	1.47	1.31
2	A	700	EIS	C3-C4	3.43	1.48	1.31
2	B	700	EIS	C3-C4	3.51	1.48	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	700	EIS	C3-C4	3.52	1.48	1.31
2	D	700	EIS	O2-C18	9.52	1.43	1.23
2	E	700	EIS	O2-C18	9.77	1.43	1.23
2	B	700	EIS	O2-C18	9.83	1.43	1.23
2	A	700	EIS	O2-C18	9.84	1.43	1.23

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	700	EIS	O2-C18-N	-17.93	92.58	123.01
2	D	700	EIS	O2-C18-N	-16.62	94.81	123.01
2	A	700	EIS	O2-C18-N	-8.79	108.10	123.01
2	D	700	EIS	O2-C18-C19	-7.56	108.94	121.98
2	B	700	EIS	O2-C18-C19	-7.53	109.00	121.98
2	E	700	EIS	O2-C18-C19	-7.46	109.12	121.98
2	A	700	EIS	O2-C18-C19	-7.13	109.68	121.98
2	E	700	EIS	O2-C18-N	-4.91	114.67	123.01
2	A	700	EIS	C5-C4-C3	-2.02	119.09	125.14
2	A	700	EIS	C46-C45-C44	2.01	113.53	110.89
2	E	700	EIS	C-O-C43	2.17	118.37	113.82
2	D	700	EIS	O4-C45-C46	2.60	114.20	108.43
2	E	700	EIS	O-C43-C44	2.82	111.59	108.04
2	A	700	EIS	O4-C45-C44	2.93	114.94	108.43
2	D	700	EIS	O4-C45-C44	3.01	115.11	108.43
2	A	700	EIS	C-O-C43	3.09	120.31	113.82
2	A	700	EIS	O-C43-C44	3.95	113.03	108.04
2	E	700	EIS	C1-N-C18	4.55	132.04	123.61
2	A	700	EIS	O4-C45-C46	4.66	118.78	108.43
2	B	700	EIS	O4-C45-C44	4.72	118.91	108.43
2	E	700	EIS	O4-C45-C46	5.38	120.39	108.43
2	B	700	EIS	O4-C45-C46	5.55	120.76	108.43
2	D	700	EIS	C45-O4-S	7.33	132.74	118.77
2	A	700	EIS	C45-O4-S	7.48	133.01	118.77
2	D	700	EIS	C-O-C43	8.34	131.35	113.82
2	A	700	EIS	C1-N-C18	8.86	140.03	123.61
2	B	700	EIS	C45-O4-S	9.00	135.91	118.77
2	B	700	EIS	C-O-C43	9.02	132.76	113.82
2	E	700	EIS	C45-O4-S	9.92	137.66	118.77
2	A	700	EIS	C19-C18-N	10.00	132.14	115.83
2	E	700	EIS	C19-C18-N	11.15	134.01	115.83
2	B	700	EIS	C1-N-C18	11.42	144.75	123.61
2	D	700	EIS	C1-N-C18	17.83	156.64	123.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	700	EIS	C19-C18-N	23.54	154.22	115.83
2	B	700	EIS	C19-C18-N	24.28	155.43	115.83

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	700	EIS	S-O4-C45-C46

There are no ring outliers.

4 monomers are involved in 32 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	700	EIS	5	0
2	B	700	EIS	5	0
2	D	700	EIS	15	0
2	E	700	EIS	16	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(Å²)	Q<0.9
1	A	209/209 (100%)	-0.32	4 (1%)	70	69	17, 29, 48, 58	0
1	B	207/209 (99%)	-0.14	6 (2%)	55	54	21, 34, 58, 82	0
1	D	206/209 (98%)	-0.01	9 (4%)	38	39	20, 37, 53, 68	0
1	E	208/209 (99%)	-0.17	4 (1%)	70	69	19, 34, 50, 56	0
All	All	830/836 (99%)	-0.16	23 (2%)	56	55	17, 33, 53, 82	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	2	ALA	5.4
1	D	170	ASN	4.3
1	D	174[A]	GLU	4.3
1	B	7	HIS	4.3
1	A	168	GLY	4.2
1	D	173	GLU	4.2
1	B	6	GLU	3.5
1	B	80	MET	3.3
1	A	2	ALA	3.1
1	D	169	GLN	3.1
1	B	5	ALA	3.0
1	D	175	GLU	3.0
1	B	168	GLY	2.9
1	E	118	GLU	2.7
1	D	83	ALA	2.7
1	A	169	GLN	2.4
1	D	38	GLY	2.3
1	D	6	GLU	2.3
1	B	79	GLU	2.3
1	E	119	ASN	2.3
1	E	168	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	73	ILE	2.1
1	A	170	ASN	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å^2)	Q<0.9
2	EIS	E	700	45/49	0.87	0.19	1.72	35,49,61,61	0
2	EIS	D	700	49/49	0.92	0.16	0.44	39,52,58,61	0
2	EIS	B	700	49/49	0.95	0.11	-0.31	28,34,43,45	0
2	EIS	A	700	49/49	0.97	0.10	-0.73	21,32,42,44	0

6.5 Other polymers (i)

There are no such residues in this entry.