



Full wwPDB X-ray Structure Validation Report ⓘ

May 20, 2025 – 04:12 AM EDT

PDB ID : 3HD7 / pdb_00003hd7
Title : HELICAL EXTENSION OF THE NEURONAL SNARE COMPLEX INTO
THE MEMBRANE, spacegroup C 1 2 1
Authors : Stein, A.; Weber, G.; Wahl, M.C.; Jahn, R.
Deposited on : 2009-05-07
Resolution : 3.40 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 Phenix2.0rc1
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0rc1
EDS : 3.0
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.006 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.43.1

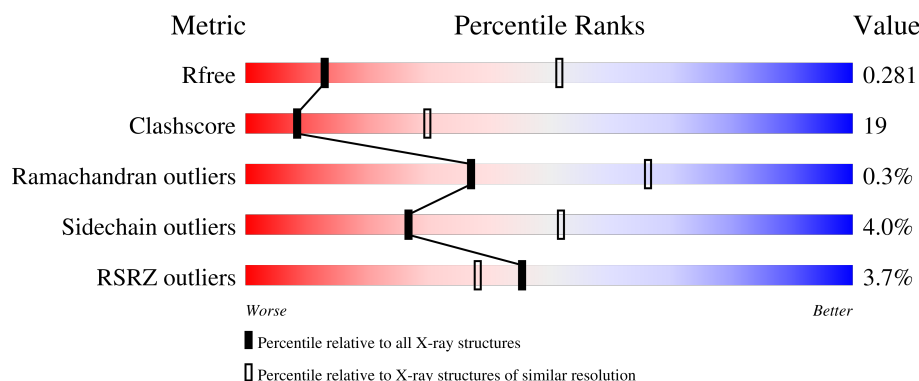
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	1140 (3.46-3.34)
Clashscore	180529	1172 (3.46-3.34)
Ramachandran outliers	177936	1172 (3.46-3.34)
Sidechain outliers	177891	1172 (3.46-3.34)
RSRZ outliers	164620	1140 (3.46-3.34)

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	91	
1	E	91	
2	B	109	
2	F	109	
3	C	80	

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Mol	Chain	Length	Quality of chain	
3	G	80		
4	D	68		
4	H	68		

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 5322 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 Vesicle-associated membrane protein 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	91	Total	C	N	O	S	0	0	0
			733	467	129	132	5			
1	E	90	Total	C	N	O	S	0	0	0
			726	463	128	130	5			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	26	GLY	-	expression tag	UNP P63045
A	27	SER	-	expression tag	UNP P63045
A	28	HIS	-	expression tag	UNP P63045
A	29	MET	-	expression tag	UNP P63045
E	26	GLY	-	expression tag	UNP P63045
E	27	SER	-	expression tag	UNP P63045
E	28	HIS	-	expression tag	UNP P63045
E	29	MET	-	expression tag	UNP P63045

- Molecule 2 is a protein called Syntaxin-1A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	98	Total	C	N	O	S	0	0	0
			779	490	135	146	8			
2	F	99	Total	C	N	O	S	0	0	0
			785	493	136	148	8			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	180	GLY	-	expression tag	UNP P32851
B	181	SER	-	expression tag	UNP P32851
B	182	HIS	-	expression tag	UNP P32851
F	180	GLY	-	expression tag	UNP P32851

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Chain	Residue	Modelled	Actual	Comment	Reference
F	181	SER	-	expression tag	UNP P32851
F	182	HIS	-	expression tag	UNP P32851

- Molecule 3 is a protein called Synaptosomal-associated protein 25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	75	Total	C	N	O	S	0	0	0
			607	360	112	130	5			
3	G	76	Total	C	N	O	S	0	0	0
			615	365	113	131	6			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	4	GLY	-	expression tag	UNP P60881
C	5	SER	-	expression tag	UNP P60881
C	6	HIS	-	expression tag	UNP P60881
G	4	GLY	-	expression tag	UNP P60881
G	5	SER	-	expression tag	UNP P60881
G	6	HIS	-	expression tag	UNP P60881

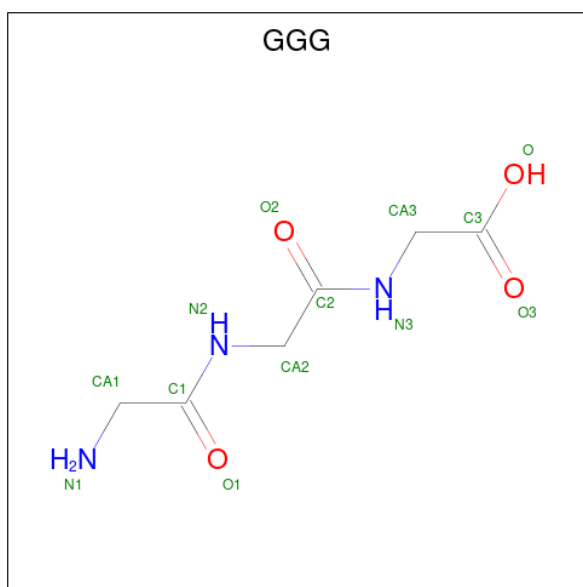
- Molecule 4 is a protein called Synaptosomal-associated protein 25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	63	Total	C	N	O	S	0	0	0
			502	293	98	106	5			
4	H	62	Total	C	N	O	S	0	0	0
			496	290	97	104	5			

There are 8 discrepancies between the modelled and reference sequences:

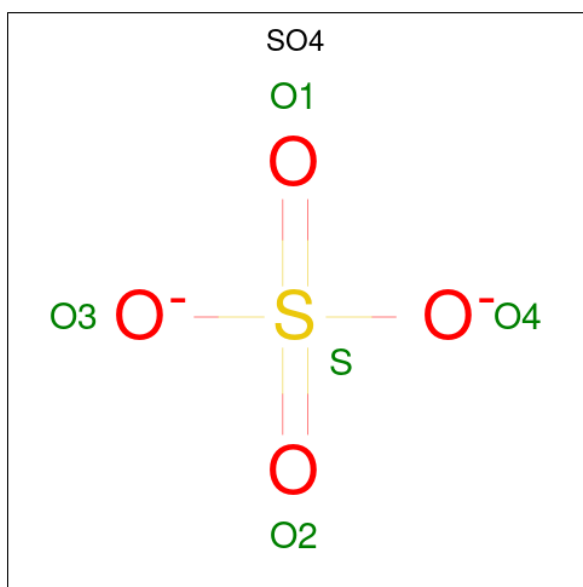
Chain	Residue	Modelled	Actual	Comment	Reference
D	137	GLY	-	expression tag	UNP P60881
D	138	SER	-	expression tag	UNP P60881
D	139	HIS	-	expression tag	UNP P60881
D	140	MET	-	expression tag	UNP P60881
H	137	GLY	-	expression tag	UNP P60881
H	138	SER	-	expression tag	UNP P60881
H	139	HIS	-	expression tag	UNP P60881
H	140	MET	-	expression tag	UNP P60881

- Molecule 5 is glycylglycylglycine (CCD ID: GGG) (formula: C₆H₁₁N₃O₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			13	6	3	4		
5	A	1	Total	C	N	O	0	0
			13	6	3	4		
5	E	1	Total	C	N	O	0	0
			13	6	3	4		

- Molecule 6 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	C	1	Total	O S	0	0
			5	4 1		

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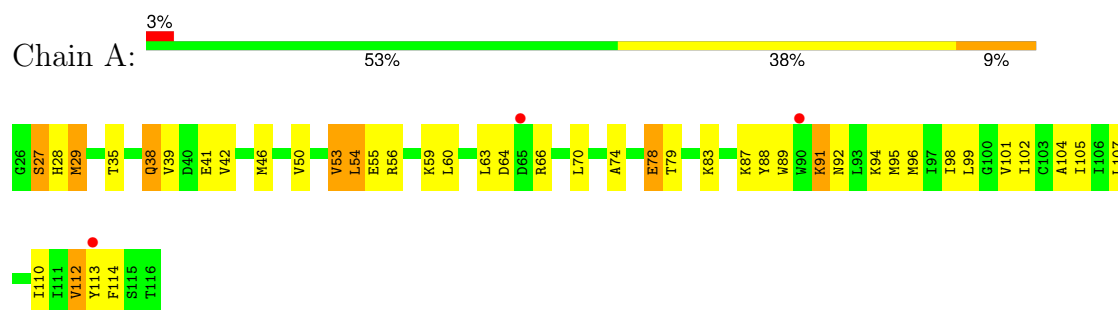
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	D	1	Total	O	S	0	0
			5	4	1		
6	E	1	Total	O	S	0	0
			5	4	1		
6	E	1	Total	O	S	0	0
			5	4	1		
6	F	1	Total	O	S	0	0
			5	4	1		
6	F	1	Total	O	S	0	0
			5	4	1		
6	F	1	Total	O	S	0	0
			5	4	1		
6	H	1	Total	O	S	0	0
			5	4	1		

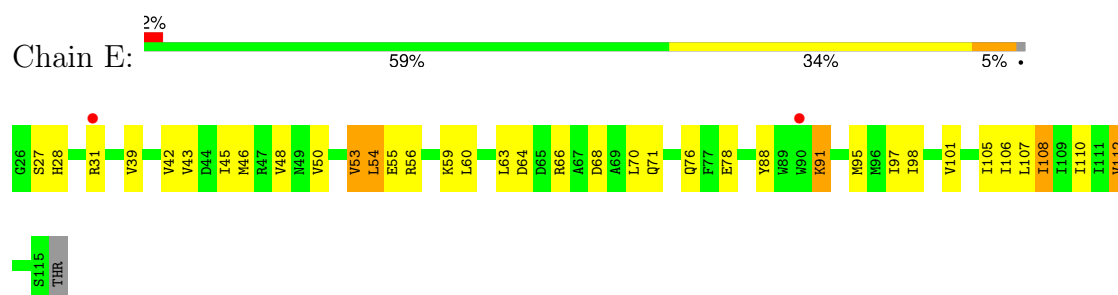
3 Residue-property plots [i](#)

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.

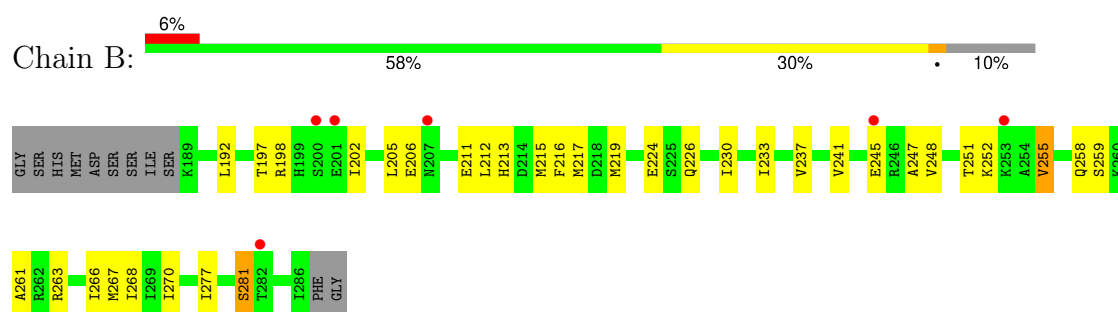
- Molecule 1: Vesicle-associated membrane protein 2



- Molecule 1: Vesicle-associated membrane protein 2

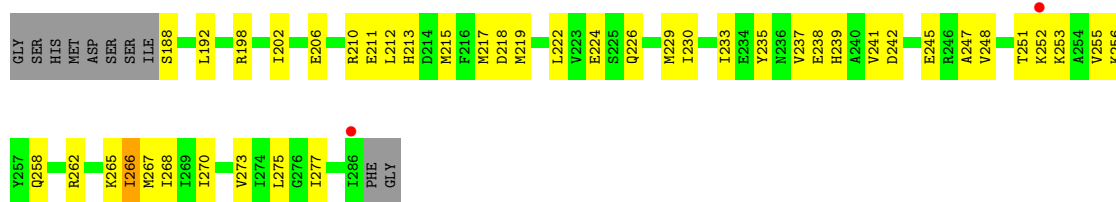


- Molecule 2: Syntaxin-1A



- Molecule 2: Syntaxin-1A

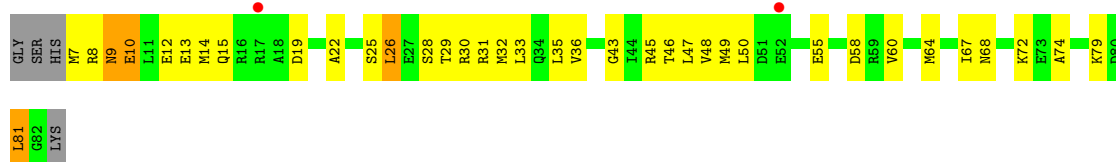




• Molecule 3: Synaptosomal-associated protein 25



• Molecule 3: Synaptosomal-associated protein 25



• Molecule 4: Synaptosomal-associated protein 25



• Molecule 4: Synaptosomal-associated protein 25



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	265.41Å 135.49Å 58.69Å 90.00° 96.34° 90.00°	Depositor
Resolution (Å)	44.20 – 3.40 44.20 – 3.40	Depositor EDS
% Data completeness (in resolution range)	98.2 (44.20-3.40) 98.7 (44.20-3.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.67 (at 3.40Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.4_4)	Depositor
R, R_{free}	0.239 , 0.271 0.241 , 0.281	Depositor DCC
R_{free} test set	1423 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	108.8	Xtriage
Anisotropy	0.447	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 168.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5322	wwPDB-VP
Average B, all atoms (Å ²)	174.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.85% 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: SO4, GGG

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	0.36	0/741	0.80	2/996 (0.2%)
1	E	0.31	0/734	0.77	0/986
2	B	0.33	0/785	0.70	0/1049
2	F	0.31	0/791	0.75	0/1057
3	C	0.31	0/607	0.73	0/807
3	G	0.29	0/615	0.74	0/817
4	D	0.30	0/503	0.75	0/671
4	H	0.30	0/497	0.79	0/663
All	All	0.31	0/5273	0.75	2/7046 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	29	MET	N-CA-C	-5.17	108.72	114.62
1	A	27	SER	N-CA-C	-5.01	106.67	112.89

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	733	0	768	44	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	726	0	761	32	0
2	B	779	0	815	31	0
2	F	785	0	820	44	0
3	C	607	0	592	28	0
3	G	615	0	601	46	0
4	D	502	0	480	23	0
4	H	496	0	475	32	0
5	A	26	0	20	4	0
5	E	13	0	10	1	0
6	C	5	0	0	0	0
6	D	5	0	0	0	0
6	E	10	0	0	0	0
6	F	15	0	0	0	0
6	H	5	0	0	0	0
All	All	5322	0	5342	199	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 19.

All (199) 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)
4:H:139:HIS:HB3	4:H:142:ARG:HH21	1.28	0.96
2:F:255:VAL:HG12	3:G:81:LEU:HD13	1.54	0.87
2:B:224:GLU:HA	3:C:49:MET:HE1	1.56	0.87
3:G:29:THR:HA	3:G:32:MET:HE3	1.59	0.83
4:H:139:HIS:HB3	4:H:142:ARG:NH2	1.93	0.83
3:G:72:LYS:HG2	4:H:191:ARG:HH21	1.41	0.83
3:G:64:MET:HE2	4:H:185:ALA:HA	1.62	0.82
4:D:139:HIS:HB3	4:D:142:ARG:HH21	1.42	0.81
2:F:224:GLU:HA	3:G:49:MET:HE1	1.63	0.81
1:A:35:THR:HG22	2:B:205:LEU:HD11	1.63	0.79
3:G:26:LEU:O	3:G:29:THR:HG22	1.85	0.76
1:A:56:ARG:O	1:A:60:LEU:HB2	1.86	0.76
1:A:42:VAL:HG12	2:B:212:LEU:HD11	1.66	0.76
1:E:27:SER:O	1:E:31:ARG:HG3	1.86	0.75
3:C:72:LYS:HG2	4:D:191:ARG:HH21	1.50	0.75
2:B:255:VAL:HG12	3:C:81:LEU:HD11	1.68	0.75
3:C:26:LEU:O	3:C:29:THR:HG22	1.86	0.75
1:E:64:ASP:HA	2:F:233:ILE:HG12	1.68	0.75
1:A:88:TYR:CD1	2:B:258:GLN:HB2	2.23	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:112:VAL:HG11	1:E:98:ILE:HD11	1.68	0.74
2:B:219:MET:HG3	3:C:46:THR:HG21	1.71	0.72
2:F:202:ILE:HD13	4:H:146:MET:HE1	1.73	0.71
2:B:255:VAL:HG12	3:C:81:LEU:CD1	2.21	0.71
1:A:87:LYS:HG2	1:A:88:TYR:CD2	2.26	0.70
2:B:245:GLU:O	2:B:248:VAL:HG12	1.92	0.68
1:A:63:LEU:HD13	4:D:182:MET:HG3	1.76	0.67
2:B:211:GLU:O	2:B:215:MET:HG2	1.95	0.66
3:G:33:LEU:HD22	4:H:149:ASN:HB2	1.78	0.66
1:A:78:GLU:HA	2:B:247:ALA:HB2	1.77	0.66
1:E:97:ILE:O	1:E:101:VAL:HG23	1.95	0.66
2:B:251:THR:O	2:B:255:VAL:HG13	1.96	0.66
4:H:177:GLN:HG3	4:H:180:ARG:NH2	2.11	0.66
2:F:211:GLU:O	2:F:215:MET:HG2	1.97	0.65
1:E:106:ILE:HG12	2:F:275:LEU:HD21	1.79	0.65
2:F:245:GLU:O	2:F:248:VAL:HG12	1.96	0.65
3:G:26:LEU:O	3:G:30:ARG:HG3	1.97	0.65
1:A:107:LEU:O	1:A:110:ILE:HG22	1.97	0.64
2:F:252:LYS:O	2:F:255:VAL:HG22	1.98	0.63
1:E:56:ARG:O	1:E:60:LEU:HB2	1.98	0.63
1:E:95:MET:HE3	2:F:268:ILE:HD12	1.80	0.63
5:A:117:GGG:N1	5:A:117:GGG:HA2A	2.13	0.63
1:A:64:ASP:HA	2:B:233:ILE:HG12	1.79	0.63
1:E:60:LEU:HD11	2:F:230:ILE:HG12	1.81	0.62
2:F:251:THR:O	2:F:255:VAL:HG13	1.99	0.62
2:F:255:VAL:HG12	3:G:81:LEU:CD1	2.26	0.62
2:B:213:HIS:NE2	2:B:217:MET:HE2	2.15	0.62
2:B:213:HIS:HA	3:C:39:SER:OG	2.00	0.62
4:D:177:GLN:HG3	4:D:180:ARG:NH2	2.15	0.61
1:A:89:TRP:HE1	5:A:117:GGG:HA2A	1.66	0.60
2:F:247:ALA:O	2:F:251:THR:HG23	2.01	0.60
2:F:219:MET:HG3	3:G:46:THR:HG21	1.83	0.59
2:F:253:LYS:O	2:F:256:LYS:HB3	2.02	0.59
3:G:22:ALA:C	4:H:142:ARG:HD2	2.28	0.59
3:G:8:ARG:C	3:G:10:GLU:H	2.11	0.59
2:F:248:VAL:HG23	3:G:74:ALA:HB2	1.85	0.58
2:B:206:GLU:OE1	3:C:28:SER:HB2	2.03	0.58
3:C:64:MET:HE2	4:D:185:ALA:HA	1.85	0.58
1:E:108:ILE:O	1:E:112:VAL:HG12	2.02	0.58
1:A:39:VAL:HG23	4:D:157:ILE:HD13	1.85	0.57
3:G:46:THR:O	3:G:50:LEU:HG	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:26:LEU:HD12	4:D:146:MET:HB3	1.85	0.57
2:F:241:VAL:HG22	3:G:67:ILE:HG13	1.87	0.57
2:B:277:ILE:O	2:B:281:SER:HB2	2.05	0.57
3:C:25:SER:HB3	4:D:146:MET:HE1	1.86	0.57
4:H:143:GLU:HA	4:H:146:MET:HG2	1.85	0.57
1:E:50:VAL:O	1:E:54:LEU:HB2	2.04	0.56
2:F:258:GLN:OE1	3:G:81:LEU:HD12	2.06	0.56
3:C:26:LEU:O	3:C:30:ARG:HG3	2.05	0.56
3:C:45:ARG:O	3:C:48:VAL:HG12	2.06	0.56
1:A:94:LYS:O	1:A:98:ILE:HG13	2.06	0.56
1:A:53:VAL:HG23	4:D:171:ILE:HD13	1.88	0.55
2:B:252:LYS:O	2:B:255:VAL:HG22	2.06	0.55
1:A:55:GLU:O	1:A:59:LYS:HG2	2.06	0.55
1:E:42:VAL:HG12	2:F:212:LEU:HD11	1.88	0.55
1:E:39:VAL:O	1:E:43:VAL:HG23	2.06	0.55
2:F:237:VAL:O	2:F:241:VAL:HG23	2.08	0.54
4:H:153:VAL:O	4:H:157:ILE:HG13	2.07	0.54
4:H:139:HIS:HA	4:H:142:ARG:HB3	1.90	0.54
1:E:107:LEU:HA	1:E:110:ILE:HG22	1.90	0.54
3:C:33:LEU:HD22	4:D:149:ASN:HB2	1.90	0.54
1:E:76:GLN:CD	4:H:196:ASN:HD21	2.15	0.54
3:C:26:LEU:HD21	3:C:30:ARG:NH2	2.23	0.54
2:F:202:ILE:CD1	4:H:146:MET:HE1	2.37	0.54
2:B:237:VAL:O	2:B:241:VAL:HG23	2.09	0.53
3:C:26:LEU:HD21	3:C:30:ARG:HH21	1.73	0.53
1:E:63:LEU:HD13	4:H:182:MET:HG3	1.90	0.53
3:G:47:LEU:HD11	4:H:163:MET:HG2	1.90	0.53
1:E:78:GLU:HA	2:F:247:ALA:HB2	1.91	0.53
2:F:192:LEU:HD12	3:G:14:MET:HG2	1.89	0.53
1:E:91:LYS:O	1:E:95:MET:HG2	2.08	0.53
1:E:107:LEU:O	1:E:110:ILE:HG22	2.09	0.53
1:A:56:ARG:HG3	4:D:175:ASN:OD1	2.08	0.53
1:A:105:ILE:HD13	1:E:105:ILE:HD11	1.91	0.53
1:A:50:VAL:O	1:A:54:LEU:HB2	2.09	0.53
1:A:91:LYS:O	1:A:95:MET:HG2	2.09	0.52
2:F:192:LEU:CD1	3:G:14:MET:HG2	2.39	0.52
1:A:74:ALA:O	1:A:78:GLU:HB2	2.10	0.52
1:E:95:MET:HE2	2:F:265:LYS:HB2	1.93	0.51
4:H:187:SER:O	4:H:191:ARG:HB2	2.10	0.51
3:G:9:ASN:O	3:G:12:GLU:N	2.43	0.51
1:A:112:VAL:HG13	1:A:113:TYR:CD2	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:28:SER:HA	3:C:31:ARG:HE	1.76	0.51
2:F:235:TYR:O	2:F:238:GLU:HB3	2.11	0.51
3:C:31:ARG:O	3:C:35:LEU:HG	2.11	0.51
3:G:45:ARG:O	3:G:49:MET:HG3	2.11	0.51
1:E:53:VAL:HG23	4:H:171:ILE:HD13	1.92	0.50
3:G:26:LEU:HD21	3:G:30:ARG:HH21	1.76	0.50
1:A:42:VAL:HG22	4:D:161:ARG:HB2	1.92	0.50
1:A:79:THR:O	1:A:83:LYS:HG3	2.11	0.50
4:D:143:GLU:HA	4:D:146:MET:HG2	1.92	0.50
4:D:152:GLN:O	4:D:156:ILE:HG13	2.12	0.50
1:E:56:ARG:HG3	4:H:175:ASN:OD1	2.11	0.50
3:G:22:ALA:HB1	4:H:142:ARG:HD2	1.94	0.50
1:A:89:TRP:HE1	5:A:117:GGG:CA2	2.25	0.50
3:G:29:THR:HA	3:G:32:MET:CE	2.37	0.49
1:A:66:ARG:O	1:A:70:LEU:HB2	2.13	0.49
2:F:267:MET:HA	2:F:270:ILE:HD12	1.93	0.49
1:E:28:HIS:HB2	2:F:198:ARG:NH2	2.28	0.49
2:F:262:ARG:O	2:F:266:ILE:HG13	2.13	0.48
3:G:60:VAL:HG12	4:H:181:ILE:HD13	1.95	0.48
1:A:66:ARG:NH1	4:D:186:ASP:HB2	2.28	0.48
3:G:19:ASP:O	3:G:22:ALA:HB3	2.14	0.48
3:G:9:ASN:O	3:G:10:GLU:C	2.57	0.48
3:G:25:SER:HB3	4:H:146:MET:HE1	1.96	0.47
3:G:26:LEU:HB2	4:H:146:MET:HB3	1.96	0.47
3:C:27:GLU:O	3:C:31:ARG:HG3	2.14	0.47
2:B:259:SER:O	2:B:263:ARG:HG3	2.15	0.47
3:C:47:LEU:HD21	4:D:167:MET:HB2	1.97	0.47
1:A:104:ALA:O	1:A:107:LEU:HB3	2.15	0.47
3:G:26:LEU:O	3:G:26:LEU:HG	2.13	0.47
3:G:7:MET:HA	3:G:13:GLU:OE1	2.16	0.46
1:A:99:LEU:HD13	2:B:268:ILE:HG13	1.97	0.46
2:F:188:SER:N	3:G:15:GLN:HE21	2.13	0.46
3:C:49:MET:HE2	3:C:53:GLN:NE2	2.30	0.46
1:A:113:TYR:O	1:A:114:PHE:CD2	2.68	0.46
1:A:27:SER:C	1:A:29:MET:H	2.24	0.46
1:A:28:HIS:CB	2:B:198:ARG:CZ	2.94	0.46
2:B:267:MET:HA	2:B:270:ILE:HD12	1.98	0.46
1:E:66:ARG:O	1:E:70:LEU:HB2	2.16	0.46
3:G:43:GLY:O	3:G:47:LEU:HG	2.15	0.45
3:C:45:ARG:O	3:C:49:MET:HG3	2.16	0.45
2:F:206:GLU:OE1	3:G:28:SER:HB2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:46:MET:O	1:A:50:VAL:HG23	2.17	0.45
2:F:192:LEU:HD23	2:F:192:LEU:O	2.17	0.45
1:E:88:TYR:CD1	2:F:258:GLN:HB2	2.52	0.45
4:H:152:GLN:O	4:H:153:VAL:C	2.60	0.45
1:E:55:GLU:O	1:E:59:LYS:HG2	2.16	0.45
1:E:43:VAL:HG22	2:F:212:LEU:HD13	1.98	0.45
1:E:68:ASP:O	1:E:71:GLN:HG3	2.17	0.45
1:A:56:ARG:NH2	4:D:174:GLN:OE1	2.48	0.44
3:G:31:ARG:O	3:G:35:LEU:HG	2.17	0.44
3:G:33:LEU:HD21	4:H:152:GLN:OE1	2.17	0.44
2:F:273:VAL:O	2:F:277:ILE:HG13	2.16	0.44
3:G:79:LYS:C	3:G:81:LEU:H	2.24	0.44
3:C:26:LEU:HB2	4:D:146:MET:HB3	1.99	0.44
2:F:218:ASP:O	2:F:222:LEU:HD13	2.17	0.44
1:A:107:LEU:HA	1:A:110:ILE:HG22	2.01	0.43
2:B:219:MET:HG2	4:D:167:MET:SD	2.58	0.43
2:F:213:HIS:NE2	2:F:217:MET:HE2	2.33	0.43
1:E:46:MET:HB2	2:F:215:MET:HE3	2.01	0.43
2:B:212:LEU:O	2:B:216:PHE:HD1	2.01	0.43
2:F:210:ARG:HG2	3:G:35:LEU:HD13	2.01	0.43
1:A:89:TRP:HE1	5:A:117:GGG:HN3	1.66	0.43
2:F:229:MET:O	2:F:233:ILE:HG13	2.19	0.43
2:B:226:GLN:O	2:B:230:ILE:HG13	2.19	0.42
1:A:29:MET:CE	2:B:197:THR:HG22	2.49	0.42
3:C:55:GLU:O	3:C:58:ASP:HB2	2.20	0.42
1:E:76:GLN:NE2	4:H:196:ASN:HD21	2.17	0.42
3:G:68:ASN:O	3:G:72:LYS:HG3	2.19	0.42
3:G:26:LEU:HD11	4:H:145:GLU:CD	2.45	0.42
2:F:253:LYS:O	2:F:256:LYS:N	2.53	0.42
1:A:92:ASN:HA	2:B:261:ALA:HB2	2.02	0.42
1:A:38:GLN:O	1:A:41:GLU:HB3	2.18	0.42
1:A:99:LEU:HA	1:A:102:ILE:HG22	2.01	0.42
3:G:64:MET:HE2	4:H:185:ALA:CA	2.42	0.42
4:H:141:ALA:O	4:H:145:GLU:N	2.52	0.42
1:E:70:LEU:HD12	1:E:70:LEU:HA	1.87	0.42
1:A:63:LEU:HD23	2:B:233:ILE:HD13	2.02	0.41
4:D:161:ARG:O	4:D:162:HIS:C	2.63	0.41
3:C:26:LEU:O	3:C:26:LEU:HG	2.19	0.41
1:E:45:ILE:O	1:E:48:VAL:HB	2.21	0.41
4:H:146:MET:HE3	4:H:146:MET:HB2	1.81	0.41
1:A:39:VAL:CG2	4:D:157:ILE:HD13	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:192:LEU:HD23	2:B:192:LEU:O	2.19	0.41
3:G:33:LEU:CD2	4:H:149:ASN:HB2	2.49	0.41
1:A:96:MET:HE2	1:A:96:MET:HB3	1.72	0.41
1:A:88:TYR:HD1	2:B:258:GLN:HB2	1.82	0.41
2:B:255:VAL:HG12	3:C:81:LEU:HD13	2.01	0.41
3:G:22:ALA:HB1	4:H:142:ARG:NE	2.36	0.41
3:G:32:MET:O	3:G:36:VAL:HG23	2.21	0.40
1:A:70:LEU:HD12	1:A:70:LEU:HA	1.81	0.40
3:C:17:ARG:O	3:C:21:LEU:HG	2.21	0.40
5:E:1:GGG:C3	2:F:262:ARG:NH1	2.85	0.40
2:F:239:HIS:O	2:F:242:ASP:N	2.54	0.40
3:G:22:ALA:HB1	4:H:142:ARG:CD	2.51	0.40
3:C:39:SER:HB3	4:D:160:LEU:HD21	2.03	0.40
4:D:152:GLN:O	4:D:153:VAL:C	2.64	0.40
2:F:222:LEU:O	2:F:226:GLN:HG3	2.21	0.40
3:G:55:GLU:O	3:G:58:ASP:HB2	2.21	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	89/91 (98%)	80 (90%)	9 (10%)	0	100	100
1	E	88/91 (97%)	81 (92%)	6 (7%)	1 (1%)	12	37
2	B	96/109 (88%)	93 (97%)	3 (3%)	0	100	100
2	F	97/109 (89%)	91 (94%)	6 (6%)	0	100	100
3	C	73/80 (91%)	71 (97%)	2 (3%)	0	100	100
3	G	74/80 (92%)	69 (93%)	4 (5%)	1 (1%)	9	31
4	D	61/68 (90%)	60 (98%)	1 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	H	60/68 (88%)	57 (95%)	3 (5%)	0	100	100
All	All	638/696 (92%)	602 (94%)	34 (5%)	2 (0%)	37	66

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	G	10	GLU
1	E	108	ILE

5.3.2 Protein sidechains ⓘ

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	80/80 (100%)	73 (91%)	7 (9%)	8	28
1	E	79/80 (99%)	75 (95%)	4 (5%)	20	46
2	B	87/96 (91%)	83 (95%)	4 (5%)	23	49
2	F	88/96 (92%)	87 (99%)	1 (1%)	70	81
3	C	67/71 (94%)	64 (96%)	3 (4%)	23	50
3	G	68/71 (96%)	64 (94%)	4 (6%)	16	41
4	D	55/58 (95%)	55 (100%)	0	100	100
4	H	54/58 (93%)	54 (100%)	0	100	100
All	All	578/610 (95%)	555 (96%)	23 (4%)	27	52

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	GLN
1	A	53	VAL
1	A	54	LEU
1	A	78	GLU
1	A	91	LYS
1	A	101	VAL

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Mol	Chain	Res	Type
1	A	112	VAL
2	B	202	ILE
2	B	255	VAL
2	B	266	ILE
2	B	281	SER
3	C	26	LEU
3	C	29	THR
3	C	48	VAL
1	E	53	VAL
1	E	54	LEU
1	E	91	LYS
1	E	112	VAL
2	F	266	ILE
3	G	9	ASN
3	G	26	LEU
3	G	48	VAL
3	G	81	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	239	HIS
3	C	68	ASN
4	D	196	ASN
4	D	197	GLN
2	F	239	HIS
3	G	66	HIS
4	H	188	ASN
4	H	196	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

11 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	$\# Z > 2$
6	SO4	F	2	-	4,4,4	0.23	0	6,6,6	0.09	0
5	GGG	A	117	-	11,12,12	0.75	1 (9%)	11,14,14	0.93	2 (18%)
6	SO4	F	9	-	4,4,4	0.25	0	6,6,6	0.13	0
6	SO4	H	10	-	4,4,4	0.23	0	6,6,6	0.09	0
6	SO4	F	3	-	4,4,4	0.24	0	6,6,6	0.08	0
5	GGG	A	1	-	11,12,12	0.71	1 (9%)	11,14,14	1.04	2 (18%)
6	SO4	E	117	-	4,4,4	0.25	0	6,6,6	0.08	0
6	SO4	D	4	-	4,4,4	0.23	0	6,6,6	0.09	0
6	SO4	E	7	-	4,4,4	0.24	0	6,6,6	0.06	0
6	SO4	C	84	-	4,4,4	0.24	0	6,6,6	0.09	0
5	GGG	E	1	-	11,12,12	0.73	1 (9%)	11,14,14	0.96	2 (18%)

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	GGG	A	117	-	-	4/12/12/12	-
5	GGG	A	1	-	-	4/12/12/12	-
5	GGG	E	1	-	-	5/12/12/12	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	1	GGG	O-C3	-2.26	1.23	1.30
5	A	117	GGG	O-C3	-2.18	1.23	1.30
5	A	1	GGG	O-C3	-2.17	1.23	1.30

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	1	GGG	O-C3-CA3	2.23	121.29	112.81
5	E	1	GGG	O-C3-O3	-2.23	117.60	123.33
5	A	117	GGG	O-C3-O3	-2.20	117.67	123.33
5	A	1	GGG	O-C3-O3	-2.19	117.70	123.33
5	A	1	GGG	O-C3-CA3	2.18	121.08	112.81
5	A	117	GGG	O-C3-CA3	2.02	120.48	112.81

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	117	GGG	O1-C1-CA1-N1
5	A	117	GGG	N2-C1-CA1-N1
5	E	1	GGG	N2-C1-CA1-N1
5	A	1	GGG	O1-C1-N2-CA2
5	A	117	GGG	O1-C1-N2-CA2
5	E	1	GGG	O1-C1-CA1-N1
5	A	1	GGG	CA1-C1-N2-CA2
5	A	117	GGG	CA1-C1-N2-CA2
5	A	1	GGG	N3-C2-CA2-N2
5	A	1	GGG	O2-C2-CA2-N2
5	E	1	GGG	N3-C2-CA2-N2
5	E	1	GGG	O2-C2-CA2-N2
5	E	1	GGG	C2-CA2-N2-C1

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	117	GGG	4	0
5	E	1	GGG	1	0

5.7 Other polymers

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, 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	91/91 (100%)	0.10	3 (3%)	49	42	98, 160, 212, 260	0
1	E	90/91 (98%)	0.05	2 (2%)	62	53	102, 160, 212, 249	0
2	B	98/109 (89%)	0.22	6 (6%)	28	27	113, 170, 224, 258	0
2	F	99/109 (90%)	0.12	2 (2%)	64	55	112, 171, 225, 259	0
3	C	75/80 (93%)	-0.00	1 (1%)	74	66	128, 175, 267, 288	0
3	G	76/80 (95%)	-0.08	2 (2%)	57	49	134, 176, 252, 284	0
4	D	63/68 (92%)	0.12	6 (9%)	15	17	129, 175, 220, 246	0
4	H	62/68 (91%)	0.07	2 (3%)	50	42	127, 175, 214, 246	0
All	All	654/696 (93%)	0.08	24 (3%)	45	38	98, 168, 232, 288	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	D	194	GLU	3.5
4	D	138	SER	3.4
2	B	200	SER	3.3
2	B	245	GLU	3.2
1	A	65	ASP	3.2
1	E	90	TRP	3.2
2	F	286	ILE	3.0
3	G	52	GLU	2.7
3	C	21	LEU	2.7
4	D	199	ALA	2.7
1	A	113	TYR	2.5
4	D	139	HIS	2.4
1	A	90	TRP	2.4
2	B	282	THR	2.4
1	E	31	ARG	2.3
2	B	201	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
2	B	207	ASN	2.2
2	B	253	LYS	2.2
4	H	140	MET	2.1
4	H	175	ASN	2.1
2	F	252	LYS	2.1
4	D	162	HIS	2.1
4	D	140	MET	2.1
3	G	17	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, 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
6	SO4	C	84	5/5	0.37	0.10	314,318,320,320	0
5	GGG	A	1	13/13	0.56	0.15	87,223,249,249	0
6	SO4	D	4	5/5	0.67	0.10	236,248,257,260	0
6	SO4	E	117	5/5	0.71	0.11	194,205,208,209	0
5	GGG	E	1	13/13	0.73	0.20	149,191,205,206	0
6	SO4	H	10	5/5	0.76	0.09	215,218,235,238	0
6	SO4	F	2	5/5	0.78	0.14	193,212,220,227	0
6	SO4	E	7	5/5	0.81	0.08	214,222,231,244	0
6	SO4	F	3	5/5	0.84	0.14	198,208,212,221	0
5	GGG	A	117	13/13	0.87	0.21	119,143,165,166	0
6	SO4	F	9	5/5	0.92	0.15	103,126,159,171	0

6.5 Other polymers [i](#)

There are no such residues in this entry.