



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 06:12 AM UTC

PDB ID : 6I7S / pdb_00006i7s
Title : Microsomal triglyceride transfer protein
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Deposited on : 2018-11-17
Resolution : 2.50 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

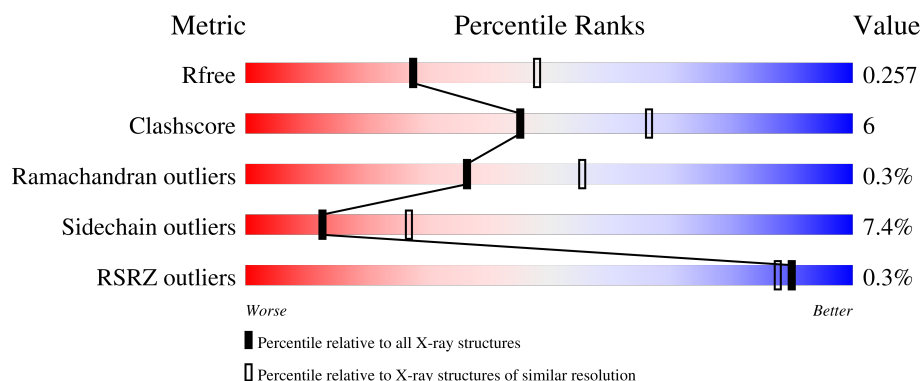
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	492	
1	B	492	
2	G	884	
2	H	884	

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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	PEG	H	917	-	-	X	-

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 21452 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 Protein disulfide-isomerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	461	Total	C	N	O	S	0	1	0
			3668	2351	602	706	9			
1	B	462	Total	C	N	O	S	0	1	0
			3676	2354	600	713	9			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	17	MET	-	initiating methionine	UNP P07237
B	17	MET	-	initiating methionine	UNP P07237

- Molecule 2 is a protein called Microsomal triglyceride transfer protein large subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	G	863	Total	C	N	O	S	0	4	0
			6787	4299	1164	1296	28			
2	H	862	Total	C	N	O	S	0	2	0
			6757	4277	1162	1290	28			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	11	MET	-	initiating methionine	UNP P55157
G	12	HIS	-	expression tag	UNP P55157
G	13	HIS	-	expression tag	UNP P55157
G	14	HIS	-	expression tag	UNP P55157
G	15	HIS	-	expression tag	UNP P55157
G	16	HIS	-	expression tag	UNP P55157
G	17	HIS	-	expression tag	UNP P55157
G	18	MET	-	expression tag	UNP P55157
H	11	MET	-	initiating methionine	UNP P55157
H	12	HIS	-	expression tag	UNP P55157

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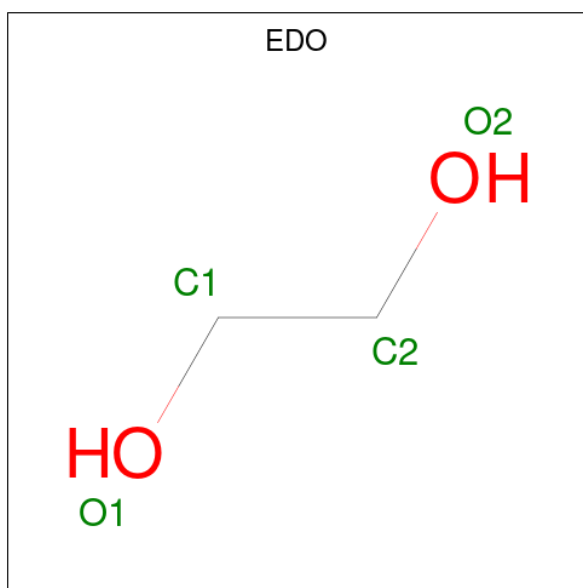
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Chain	Residue	Modelled	Actual	Comment	Reference
H	13	HIS	-	expression tag	UNP P55157
H	14	HIS	-	expression tag	UNP P55157
H	15	HIS	-	expression tag	UNP P55157
H	16	HIS	-	expression tag	UNP P55157
H	17	HIS	-	expression tag	UNP P55157
H	18	MET	-	expression tag	UNP P55157

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Ca 1 1	0	0
3	B	1	Total Ca 1 1	0	0

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	G	1	Total	C	O	0	0
			4	2	2		
4	G	1	Total	C	O	0	0
			4	2	2		
4	G	1	Total	C	O	0	0
			4	2	2		
4	G	1	Total	C	O	0	0
			4	2	2		
4	G	1	Total	C	O	0	0
			4	2	2		
4	H	1	Total	C	O	0	0
			4	2	2		
4	H	1	Total	C	O	0	0
			4	2	2		
4	H	1	Total	C	O	0	0
			4	2	2		
4	H	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: C₆H₁₄O₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			10	6	4		
5	B	1	Total	C	O	0	0
			10	6	4		
5	G	1	Total	C	O	0	0
			10	6	4		
5	H	1	Total	C	O	0	0
			10	6	4		
5	H	1	Total	C	O	0	0
			10	6	4		
5	H	1	Total	C	O	0	0
			10	6	4		

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



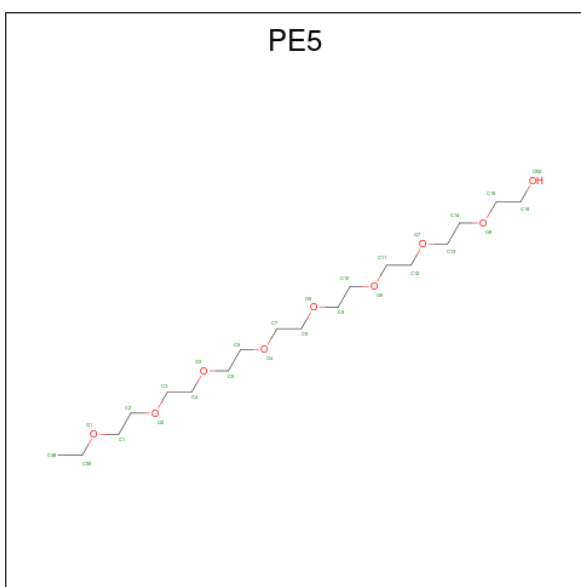
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	O	S	0	0
			5	4	1		
6	G	1	Total	O	S	0	0
			5	4	1		
6	G	1	Total	O	S	0	0
			5	4	1		
6	G	1	Total	O	S	0	0
			5	4	1		
6	G	1	Total	O	S	0	0
			5	4	1		
6	G	1	Total	O	S	0	0
			5	4	1		
6	H	1	Total	O	S	0	0
			5	4	1		
6	H	1	Total	O	S	0	0
			5	4	1		
6	H	1	Total	O	S	0	0
			5	4	1		

- Molecule 7 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C₄H₁₀O₃).



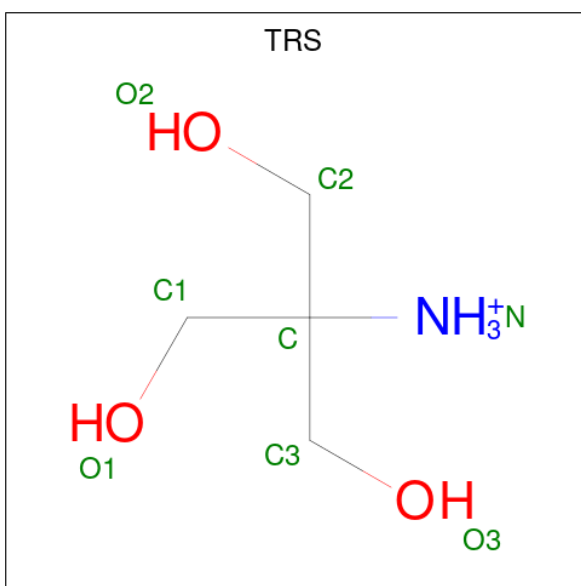
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	C	O	0	0
			7	4	3		
7	B	1	Total	C	O	0	0
			7	4	3		
7	G	1	Total	C	O	0	0
			7	4	3		
7	G	1	Total	C	O	0	0
			7	4	3		
7	H	1	Total	C	O	0	0
			7	4	3		
7	H	1	Total	C	O	0	0
			7	4	3		
7	H	1	Total	C	O	0	0
			7	4	3		
7	H	1	Total	C	O	0	0
			7	4	3		

- Molecule 8 is 3,6,9,12,15,18,21,24-OCTAOXAHEXACOSAN-1-OL (CCD ID: PE5) (formula: $C_{18}H_{38}O_9$).



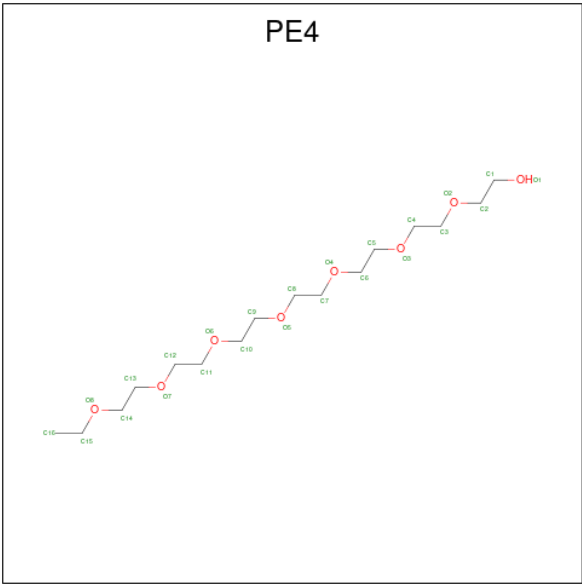
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	G	1	Total	C	O	0	0
			27	18	9		
8	H	1	Total	C	O	0	0
			27	18	9		

- Molecule 9 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (CCD ID: TRS) (formula: $\text{C}_4\text{H}_{12}\text{NO}_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	G	1	Total	C	N	O	0	0
			8	4	1	3		

- Molecule 10 is 2-{2-[2-(2-{2-[2-(2-ETHOXY-ETHOXY)-ETHOXY]-ETHOXY}-ETHOXY)-ETHOXY]-ETHOXY}-ETHANOL (CCD ID: PE4) (formula: C₁₆H₃₄O₈).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	H	1	Total	C	O	0	0
			24	16	8		

- Molecule 11 is water.

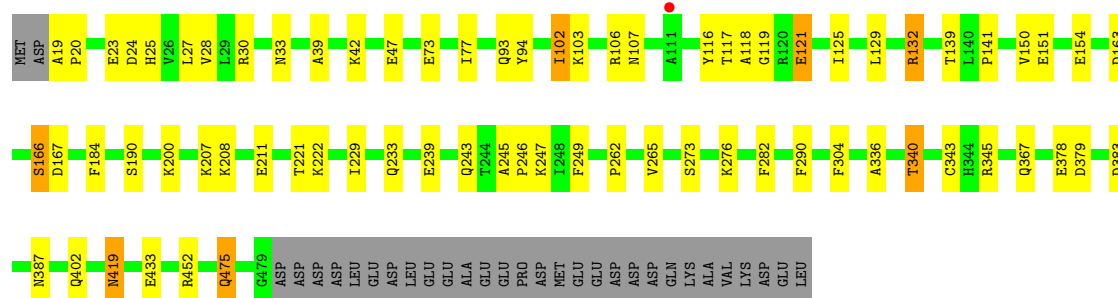
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	22	Total	O	0	0
			22	22		
11	B	32	Total	O	0	0
			32	32		
11	G	81	Total	O	0	0
			81	81		
11	H	87	Total	O	0	0
			87	87		

3 Residue-property plots

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

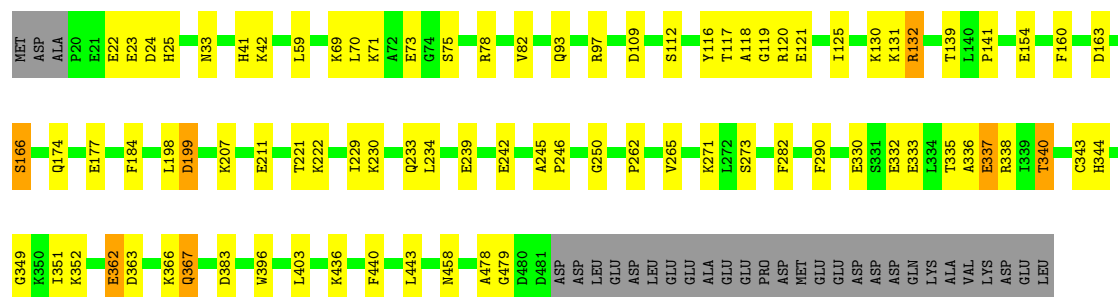
- Molecule 1: Protein disulfide-isomerase

Chain A: 



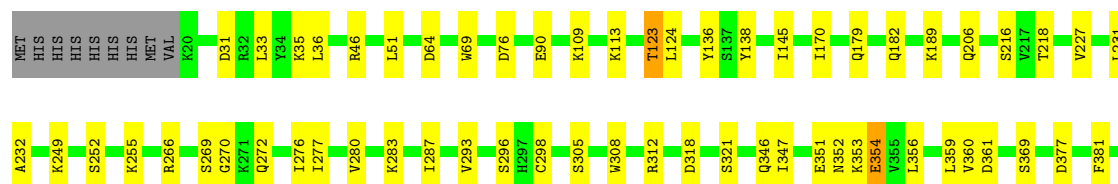
- Molecule 1: Protein disulfide-isomerase

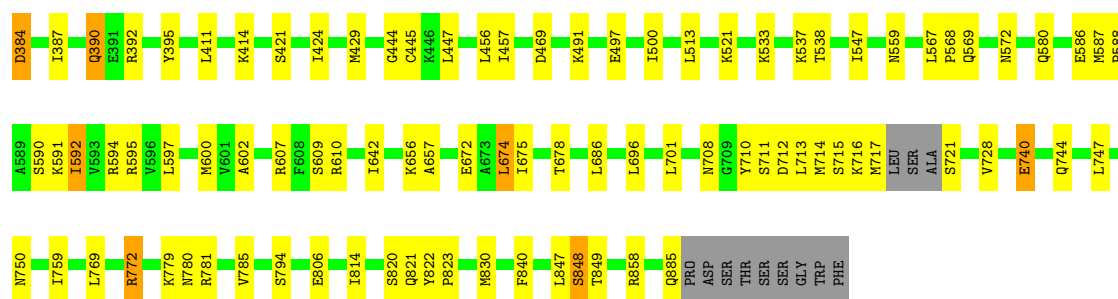
Chain B: 



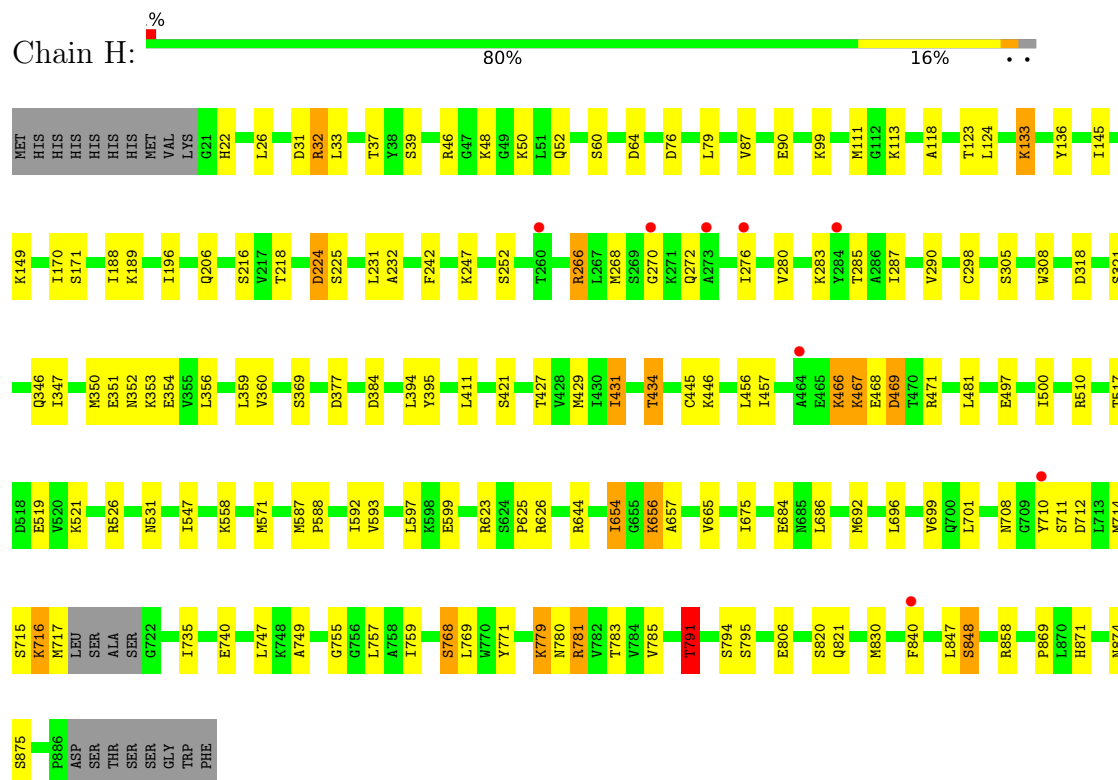
- Molecule 2: Microsomal triglyceride transfer protein large subunit

Chain G: 





• Molecule 2: Microsomal triglyceride transfer protein large subunit



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	77.54Å 105.59Å 112.27Å 89.81° 76.95° 74.24°	Depositor
Resolution (Å)	49.35 – 2.50 49.35 – 2.50	Depositor EDS
% Data completeness (in resolution range)	93.8 (49.35-2.50) 93.9 (49.35-2.50)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.07 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.204 , 0.257 0.204 , 0.257	Depositor DCC
R_{free} test set	5414 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	65.6	Xtriage
Anisotropy	0.143	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 52.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	21452	wwPDB-VP
Average B, all atoms (Å ²)	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.33% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PE4, CA, SO4, PEG, PE5, EDO, TRS, PGE

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	0/3756	1.04	3/5071 (0.1%)
1	B	0.55	0/3764	1.05	5/5082 (0.1%)
2	G	0.58	0/6897	1.04	1/9297 (0.0%)
2	H	0.57	0/6868	1.06	6/9258 (0.1%)
All	All	0.56	0/21285	1.05	15/28708 (0.1%)

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	22	HIS	CB-CA-C	6.74	117.86	109.16
1	B	33	ASN	CA-CB-CG	6.45	119.05	112.60
2	H	224	ASP	CA-CB-CG	6.30	118.90	112.60
2	H	791	THR	CA-CB-OG1	-6.14	100.39	109.60
2	H	133	LYS	CB-CA-C	5.93	119.34	109.56
1	A	383	ASP	CA-C-N	5.37	128.01	120.28
1	A	383	ASP	C-N-CA	5.37	128.01	120.28
1	B	362	GLU	CB-CA-C	5.37	119.70	110.79
1	B	352	LYS	CB-CA-C	5.32	116.52	108.86
1	B	383	ASP	CA-C-N	5.30	127.91	120.28
1	B	383	ASP	C-N-CA	5.30	127.91	120.28
1	A	345	ARG	CB-CG-CD	5.27	123.42	111.30
2	G	740	GLU	CB-CG-CD	5.17	121.40	112.60
2	H	285	THR	CB-CA-C	5.11	119.47	109.35
2	H	740	GLU	CB-CG-CD	5.04	121.17	112.60

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	3668	0	3593	36	0
1	B	3676	0	3588	41	0
2	G	6787	0	6921	88	0
2	H	6757	0	6899	91	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	20	0	30	4	0
4	B	12	0	18	0	0
4	G	24	0	36	1	0
4	H	20	0	30	0	0
5	B	20	0	28	1	0
5	G	10	0	14	5	0
5	H	30	0	42	2	0
6	B	5	0	0	0	0
6	G	35	0	0	2	0
6	H	15	0	0	1	0
7	B	14	0	20	0	0
7	G	14	0	20	0	0
7	H	35	0	50	7	0
8	G	27	0	38	1	0
8	H	27	0	38	6	0
9	G	8	0	12	1	0
10	H	24	0	34	2	0
11	A	22	0	0	0	0
11	B	32	0	0	1	0
11	G	81	0	0	4	0
11	H	87	0	0	3	0
All	All	21452	0	21411	253	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 6.

All (253) 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)
2:G:717:MET:CE	2:G:721:SER:CB	2.12	1.28
2:G:717:MET:HE3	2:G:721:SER:CB	1.71	1.20
2:G:717:MET:CE	2:G:721:SER:HB3	1.69	1.19
2:H:79:LEU:CD2	2:H:276:ILE:HD11	1.72	1.18
2:G:395:TYR:CE2	5:G:902:PGE:H22	1.92	1.04
2:H:780:ASN:ND2	8:H:901:PE5:H142	1.76	1.01
2:H:780:ASN:HD22	8:H:901:PE5:H142	1.21	1.00
2:G:717:MET:HE2	2:G:721:SER:HB2	1.44	0.99
2:G:717:MET:CE	2:G:721:SER:HB2	1.94	0.97
2:H:429:MET:HE2	2:H:457:ILE:HG12	1.50	0.94
2:G:717:MET:HE3	2:G:721:SER:HB3	0.92	0.91
2:H:79:LEU:HD23	2:H:276:ILE:HD11	1.48	0.90
2:G:587:MET:HB3	2:G:588:PRO:HD2	1.53	0.90
2:H:656:LYS:HE2	2:H:656:LYS:H	1.39	0.87
2:G:429:MET:HE2	2:G:457:ILE:HG12	1.56	0.86
2:G:822[B]:TYR:CD1	2:G:823[B]:PRO:HA	2.11	0.84
2:H:780:ASN:ND2	8:H:901:PE5:H151	1.93	0.84
2:H:587:MET:HB3	2:H:588:PRO:HD2	1.60	0.82
2:G:569:GLN:O	11:G:1001:HOH:O	1.99	0.80
2:G:717:MET:HE1	2:G:721:SER:HA	1.64	0.80
1:A:20:PRO:HG2	1:A:27:LEU:HD22	1.66	0.77
2:H:79:LEU:HD22	2:H:276:ILE:HD11	1.64	0.76
1:B:163:ASP:HB3	1:B:166:SER:HB2	1.69	0.74
2:H:79:LEU:CD2	2:H:276:ILE:CD1	2.60	0.74
2:H:79:LEU:HD23	2:H:276:ILE:CD1	2.17	0.74
1:A:163:ASP:HB3	1:A:166:SER:HB2	1.71	0.72
1:A:19:ALA:N	1:A:20:PRO:CD	2.54	0.71
2:H:466:LYS:HB2	2:H:469:ASP:HB2	1.71	0.71
1:B:41:HIS:CE1	1:B:78:ARG:HG3	2.26	0.70
2:G:270:GLY:HA3	2:G:276:ILE:HD11	1.71	0.70
2:H:352:ASN:O	2:H:356:LEU:HB2	1.90	0.70
2:G:352:ASN:O	2:G:356:LEU:HB2	1.92	0.70
2:G:444:GLY:HA2	2:G:447:LEU:HD13	1.74	0.69
1:B:22:GLU:HG2	1:B:25:HIS:HA	1.72	0.69
2:G:710:TYR:HE2	2:G:714:MET:HE3	1.56	0.69
2:G:717:MET:CE	2:G:721:SER:CA	2.71	0.68
2:H:526:ARG:HA	2:H:531:ASN:HD22	1.58	0.68
2:H:356:LEU:O	2:H:360:VAL:HG23	1.93	0.68
2:G:356:LEU:O	2:G:360:VAL:HG23	1.94	0.68
1:A:262:PRO:HG2	1:A:265:VAL:HB	1.75	0.67
1:B:458:ASN:HB2	1:B:479:GLY:H	1.60	0.67
1:B:262:PRO:HG2	1:B:265:VAL:HB	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:847:LEU:O	2:G:848:SER:HB3	1.96	0.66
2:H:847:LEU:O	2:H:848:SER:HB3	1.96	0.66
2:H:429:MET:CE	2:H:457:ILE:HG12	2.24	0.65
2:H:517:THR:HB	6:H:906:SO4:O4	1.96	0.65
2:G:227:VAL:O	9:G:903:TRS:H11	1.97	0.64
1:B:174:GLN:HB3	1:B:222:LYS:HD2	1.78	0.64
2:G:717:MET:HE1	2:G:721:SER:CA	2.28	0.63
2:H:780:ASN:HD22	8:H:901:PE5:C14	2.05	0.63
2:G:602:ALA:O	2:G:607:ARG:HD2	1.99	0.62
2:H:701:LEU:HD13	7:H:914:PEG:H42	1.82	0.62
1:A:150:VAL:HG13	4:A:603:EDO:H22	1.82	0.61
1:B:230:LYS:HA	1:B:233:GLN:HE21	1.64	0.61
1:B:458:ASN:H	1:B:478:ALA:HA	1.66	0.61
2:G:444:GLY:CA	2:G:447:LEU:HD13	2.31	0.61
1:A:276:LYS:HE2	4:A:604:EDO:O1	2.00	0.61
2:G:36:LEU:HD12	2:G:36:LEU:N	2.16	0.61
2:H:60:SER:HB2	7:H:917:PEG:H21	1.82	0.61
2:H:434:THR:HG21	2:H:699:VAL:HG22	1.83	0.61
2:G:429:MET:CE	2:G:457:ILE:HG12	2.27	0.60
2:H:429:MET:HE2	2:H:457:ILE:CG1	2.29	0.60
2:H:768:SER:HB2	2:H:771:TYR:HB2	1.83	0.60
2:H:99:LYS:NZ	10:H:902:PE4:H81	2.17	0.60
2:G:710:TYR:CE2	2:G:714:MET:HE3	2.36	0.60
2:G:390:GLN:NE2	2:G:424:ILE:HD13	2.18	0.59
1:B:242:GLU:N	1:B:242:GLU:OE1	2.35	0.59
2:H:779:LYS:HE2	2:H:781:ARG:HD2	1.84	0.58
1:A:208:LYS:HG2	4:A:603:EDO:H12	1.86	0.58
2:H:276:ILE:O	2:H:280:VAL:HG23	2.03	0.58
2:G:381:PHE:CD1	2:G:414:LYS:HE3	2.39	0.58
1:A:387:ASN:HD22	1:A:419:ASN:ND2	2.02	0.57
2:G:255:LYS:HE2	6:G:907:SO4:O1	2.04	0.57
2:G:780:ASN:HD22	8:G:901:PE5:H72	1.69	0.57
2:H:840[A]:PHE:CD1	2:H:858:ARG:HG2	2.39	0.57
2:G:822[B]:TYR:CG	2:G:823[B]:PRO:HA	2.39	0.57
2:G:429:MET:HE2	2:G:457:ILE:CG1	2.33	0.56
2:H:124:LEU:HB2	2:H:136:TYR:HB2	1.87	0.55
1:A:47:GLU:HG3	1:A:102:ILE:HD13	1.87	0.55
2:H:466:LYS:O	2:H:469:ASP:N	2.37	0.55
1:A:121:GLU:O	1:A:125:ILE:HD13	2.07	0.55
1:A:116:TYR:OH	1:A:119:GLY:O	2.23	0.55
2:G:33:LEU:HD11	2:G:64:ASP:HB3	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:840[A]:PHE:HD1	2:H:858:ARG:HG2	1.72	0.55
1:B:245:ALA:HB3	1:B:246:PRO:HD3	1.89	0.55
1:A:245:ALA:HB3	1:A:246:PRO:HD3	1.89	0.55
2:G:390:GLN:HE21	2:G:424:ILE:HG21	1.72	0.54
2:H:99:LYS:HZ1	10:H:902:PE4:H81	1.72	0.54
2:G:840[A]:PHE:HD1	2:G:858:ARG:HG2	1.73	0.54
1:B:239:GLU:HB2	1:B:290:PHE:CZ	2.43	0.54
2:G:276:ILE:O	2:G:280:VAL:HG23	2.07	0.54
2:H:37:THR:HB	7:H:917:PEG:H31	1.90	0.54
2:H:196:ILE:HD13	2:H:290:VAL:CG1	2.38	0.54
2:G:587:MET:HB3	2:G:588:PRO:CD	2.33	0.54
2:H:429:MET:CE	2:H:457:ILE:CG1	2.85	0.54
1:B:282:PHE:CZ	1:B:343:CYS:HB2	2.43	0.54
1:B:70:LEU:HD23	1:B:75:SER:HB3	1.89	0.53
2:H:48:LYS:HB2	2:H:247:LYS:NZ	2.24	0.53
1:A:378:GLU:CD	1:A:452:ARG:HH22	2.15	0.53
2:H:780:ASN:HD22	8:H:901:PE5:H151	1.67	0.53
1:B:174:GLN:O	1:B:177:GLU:HG3	2.08	0.53
1:B:121:GLU:O	1:B:125:ILE:HD13	2.08	0.53
2:G:429:MET:CE	2:G:457:ILE:CG1	2.87	0.53
2:H:196:ILE:HD13	2:H:290:VAL:HG11	1.90	0.53
2:G:124:LEU:HB2	2:G:136:TYR:HB2	1.92	0.52
1:A:184:PHE:HZ	1:A:229:ILE:HD13	1.73	0.52
1:A:282:PHE:CZ	1:A:343:CYS:HB2	2.44	0.52
1:A:239:GLU:HB2	1:A:290:PHE:CZ	2.45	0.52
1:A:30:ARG:HB3	1:A:33:ASN:HD21	1.75	0.52
2:G:580:GLN:HG2	11:G:1033:HOH:O	2.08	0.52
2:H:847:LEU:O	2:H:848:SER:CB	2.56	0.52
2:G:31:ASP:OD1	2:G:266:ARG:HA	2.10	0.52
2:H:558:LYS:NZ	2:H:599:GLU:OE2	2.43	0.52
1:A:19:ALA:N	1:A:20:PRO:HD2	2.24	0.51
1:B:458:ASN:HB2	1:B:479:GLY:N	2.24	0.51
2:H:394:LEU:HB3	2:H:431:ILE:HD13	1.93	0.51
2:H:87:VAL:HG12	2:H:111:MET:HE1	1.93	0.51
2:H:171:SER:O	2:H:196:ILE:HG21	2.11	0.51
2:H:283:LYS:HB3	11:H:1022:HOH:O	2.10	0.51
1:B:59:LEU:HD13	1:B:120:ARG:HD3	1.93	0.51
2:G:840[A]:PHE:CD1	2:G:858:ARG:HG2	2.45	0.51
1:B:184:PHE:HZ	1:B:229:ILE:HD13	1.76	0.50
2:H:785:VAL:HG22	2:H:806:GLU:HB3	1.93	0.50
2:H:710:TYR:HB3	2:H:714:MET:HE3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:26:LEU:HA	5:H:905:PGE:H1	1.93	0.50
1:A:77:ILE:HD11	1:A:132:ARG:NH1	2.27	0.50
2:H:33:LEU:HD11	2:H:64:ASP:HB3	1.94	0.49
1:A:304:PHE:HB2	2:G:609:SER:OG	2.12	0.49
2:G:592:ILE:HD12	2:G:595:ARG:NH1	2.28	0.49
1:A:190:SER:HB3	4:A:602:EDO:H22	1.93	0.48
1:B:97:ARG:NH2	1:B:250:GLY:O	2.46	0.48
2:G:701:LEU:HD13	5:G:902:PGE:H2	1.94	0.48
2:H:189:LYS:HB3	2:H:216:SER:HB3	1.95	0.48
2:G:572:ASN:HB3	2:G:610:ARG:CD	2.44	0.48
2:G:747:LEU:HD22	2:G:794:SER:HB3	1.95	0.48
1:A:475:GLN:HE21	1:A:475:GLN:N	2.12	0.48
2:H:769:LEU:C	2:H:769:LEU:HD13	2.39	0.48
2:G:572:ASN:HB3	2:G:610:ARG:HD3	1.95	0.48
2:H:48:LYS:HB2	2:H:247:LYS:HZ2	1.79	0.48
2:G:189:LYS:HB3	2:G:216:SER:HB3	1.96	0.48
2:H:39:SER:HB2	7:H:917:PEG:H42	1.96	0.48
2:H:266:ARG:H	2:H:266:ARG:HD3	1.78	0.47
2:G:308:TRP:CD1	2:G:347:ILE:HG23	2.49	0.47
2:G:769:LEU:O	2:G:772:ARG:HD3	2.15	0.47
2:G:123:THR:HG21	11:G:1040:HOH:O	2.13	0.47
2:G:296:SER:HB2	11:G:1077:HOH:O	2.12	0.47
2:G:674:LEU:HD11	2:G:713:LEU:HD21	1.95	0.47
2:H:308:TRP:CD1	2:H:347:ILE:HG23	2.49	0.47
2:G:847:LEU:O	2:G:848:SER:CB	2.56	0.47
1:A:42:LYS:O	1:A:106:ARG:O	2.32	0.47
1:A:94:TYR:O	1:A:103:LYS:HE3	2.15	0.47
1:B:116:TYR:OH	1:B:119:GLY:O	2.26	0.47
2:G:351:GLU:HB3	2:G:356:LEU:HD13	1.97	0.47
2:G:124:LEU:HD23	2:G:277:ILE:HG12	1.97	0.47
2:H:395:TYR:CD2	7:H:914:PEG:H41	2.49	0.47
2:H:521:LYS:HG2	2:H:547:ILE:HG12	1.97	0.47
1:A:249:PHE:HA	2:G:600:MET:HE2	1.98	0.46
1:B:82:VAL:HA	11:B:704:HOH:O	2.14	0.46
2:G:384:ASP:OD1	2:G:387:ILE:HD11	2.15	0.46
2:H:32:ARG:HD3	11:H:1028:HOH:O	2.15	0.46
2:H:99:LYS:HD2	2:H:99:LYS:HA	1.77	0.46
2:H:206:GLN:HB2	2:H:657:ALA:CB	2.45	0.46
2:H:747:LEU:HD22	2:H:794:SER:HB3	1.97	0.46
1:B:335:THR:OG1	1:B:337:GLU:HG2	2.15	0.46
2:H:242:PHE:HA	2:H:654:ILE:HD11	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:593:VAL:O	2:H:597:LEU:HG	2.16	0.46
2:H:171:SER:O	2:H:196:ILE:CG2	2.63	0.45
1:B:154:GLU:O	1:B:207:LYS:HA	2.16	0.45
2:G:312:ARG:HH22	4:G:915:EDO:H21	1.80	0.45
2:H:625:PRO:HG2	11:H:1048:HOH:O	2.16	0.45
2:G:785:VAL:HG22	2:G:806:GLU:HB3	1.98	0.45
2:G:51:LEU:HD11	2:G:249:LYS:HD2	1.99	0.45
1:A:30:ARG:HB3	1:A:33:ASN:ND2	2.32	0.45
2:G:521:LYS:HG2	2:G:547:ILE:HG12	1.99	0.45
1:B:336:ALA:O	1:B:340:THR:OG1	2.35	0.45
2:H:467:LYS:HE2	2:H:467:LYS:HB3	1.60	0.45
2:G:696:LEU:HD23	2:G:696:LEU:HA	1.87	0.44
2:H:467:LYS:HG2	2:H:468:GLU:OE2	2.17	0.44
1:A:336:ALA:O	1:A:340:THR:OG1	2.33	0.44
2:G:347:ILE:HG22	2:G:359:LEU:HD21	1.99	0.44
1:A:154:GLU:O	1:A:207:LYS:HA	2.17	0.44
1:B:230:LYS:HA	1:B:233:GLN:NE2	2.30	0.44
2:G:136:TYR:CZ	2:G:277:ILE:HD13	2.53	0.44
2:G:395:TYR:HE2	5:G:902:PGE:H22	1.71	0.44
2:G:708:ASN:O	2:G:712:ASP:HB3	2.17	0.44
2:H:749:ALA:HA	2:H:791:THR:O	2.18	0.44
2:G:538:THR:HG23	6:G:906:SO4:O2	2.18	0.44
1:B:363:ASP:HB2	1:B:366:LYS:HB2	1.99	0.43
2:G:769:LEU:O	2:G:772:ARG:CD	2.66	0.43
1:B:396:TRP:CH2	2:H:875:SER:HB3	2.53	0.43
2:H:587:MET:HB3	2:H:588:PRO:CD	2.42	0.43
1:A:39:ALA:HA	1:A:107:ASN:ND2	2.33	0.43
1:B:116:TYR:CZ	1:B:118:ALA:HB3	2.53	0.43
2:H:31:ASP:OD1	2:H:266:ARG:HA	2.19	0.43
2:G:138:TYR:HE1	2:G:283:LYS:HB2	1.84	0.43
2:H:37:THR:HG22	7:H:917:PEG:H12	2.00	0.43
2:H:351:GLU:HB3	2:H:356:LEU:HD13	2.01	0.43
2:H:37:THR:CG2	7:H:917:PEG:H12	2.49	0.43
1:A:139:THR:O	1:A:141:PRO:HD3	2.19	0.43
2:H:87:VAL:CG1	2:H:111:MET:HE1	2.49	0.43
2:H:526:ARG:HA	2:H:531:ASN:ND2	2.30	0.43
1:A:24:ASP:O	1:A:25:HIS:HB2	2.18	0.43
5:G:902:PGE:H2	5:G:902:PGE:H4	1.77	0.42
2:H:696:LEU:HD23	2:H:696:LEU:HA	1.88	0.42
2:G:381:PHE:CE1	2:G:414:LYS:HE3	2.54	0.42
1:A:116:TYR:CZ	1:A:118:ALA:HB3	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:735:ILE:HB	2:H:755:GLY:HA3	2.00	0.42
2:G:361:ASP:OD2	2:G:392:ARG:NH1	2.52	0.42
2:G:51:LEU:HD11	2:G:249:LYS:CD	2.49	0.42
2:G:772:ARG:HG2	2:G:820:SER:HA	2.01	0.42
2:H:347:ILE:HG22	2:H:359:LEU:HD21	2.01	0.42
2:H:481:LEU:HD21	2:H:510:ARG:HB2	2.01	0.42
1:B:367:GLN:HE21	1:B:367:GLN:HB2	1.69	0.42
2:H:780:ASN:HD21	8:H:901:PE5:H151	1.77	0.42
1:B:333:GLU:HB2	1:B:338:ARG:HG3	2.02	0.42
2:G:642:ILE:HD12	2:G:672:GLU:HG3	2.02	0.42
1:A:19:ALA:N	1:A:20:PRO:HD3	2.33	0.41
2:G:206:GLN:HB2	2:G:657:ALA:CB	2.49	0.41
1:A:47:GLU:HG3	1:A:102:ILE:CD1	2.48	0.41
1:B:139:THR:O	1:B:141:PRO:HD3	2.20	0.41
2:G:182:GLN:OE1	2:G:182:GLN:HA	2.19	0.41
2:H:218:THR:HG23	2:H:232:ALA:HB2	2.02	0.41
1:B:24:ASP:O	1:B:25:HIS:HB2	2.20	0.41
2:G:740:GLU:HG3	2:G:750:ASN:HD21	1.85	0.41
2:G:567:LEU:HB3	2:G:568:PRO:HD2	2.01	0.41
1:B:403:LEU:HD21	1:B:443:LEU:HD21	2.02	0.41
2:G:218:THR:HG23	2:G:232:ALA:HB2	2.03	0.41
2:G:352:ASN:OD1	2:G:354:GLU:HG2	2.21	0.41
1:A:129:LEU:O	1:A:132:ARG:HD3	2.19	0.41
2:G:35:LYS:C	2:G:36:LEU:HD12	2.46	0.41
2:G:456:LEU:HD12	2:G:456:LEU:HA	1.94	0.41
2:G:559:ASN:HD22	2:G:559:ASN:HA	1.67	0.41
2:H:50:LYS:C	2:H:52:GLN:H	2.29	0.41
2:G:590:SER:HB3	2:G:594:ARG:NH2	2.35	0.41
2:H:708:ASN:O	2:H:712:ASP:HB3	2.20	0.41
2:H:757:LEU:HA	2:H:783:THR:O	2.20	0.41
1:A:154:GLU:HA	1:A:208:LYS:HG3	2.03	0.41
2:G:69:TRP:CD1	2:G:276:ILE:HG13	2.56	0.41
2:H:427:THR:O	2:H:431:ILE:HD12	2.21	0.41
1:B:69:LYS:O	1:B:73:GLU:HB2	2.21	0.40
1:B:132:ARG:HD3	1:B:132:ARG:HA	1.76	0.40
1:B:349:GLY:HA2	5:B:603:PGE:H1	2.01	0.40
1:B:396:TRP:HH2	2:H:875:SER:HB3	1.85	0.40
2:G:728:VAL:HG13	5:G:902:PGE:H5	2.02	0.40
2:H:456:LEU:HD12	2:H:456:LEU:HA	1.96	0.40
1:B:160:PHE:CD1	1:B:198:LEU:CD1	3.05	0.40
2:H:118:ALA:O	2:H:149:LYS:HE2	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:665:VAL:O	2:H:692:MET:HA	2.21	0.40
1:B:199:ASP:OD1	1:B:199:ASP:N	2.54	0.40
1:B:440:PHE:CE2	2:H:869:PRO:HB3	2.56	0.40
2:H:871:HIS:CE1	2:H:874:ASN:HB2	2.56	0.40
5:H:903:PGE:H32	5:H:903:PGE:H52	1.54	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	460/492 (94%)	436 (95%)	22 (5%)	2 (0%)	30	49
1	B	461/492 (94%)	440 (95%)	19 (4%)	2 (0%)	30	49
2	G	863/884 (98%)	831 (96%)	31 (4%)	1 (0%)	48	68
2	H	860/884 (97%)	828 (96%)	28 (3%)	4 (0%)	24	43
All	All	2644/2752 (96%)	2535 (96%)	100 (4%)	9 (0%)	36	55

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	23	GLU
1	A	166	SER
1	B	23	GLU
1	B	166	SER
2	H	716	LYS
2	G	76	ASP
2	H	76	ASP
2	H	795	SER
2	H	270	GLY

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	391/419 (93%)	367 (94%)	24 (6%)	17	35
1	B	393/419 (94%)	370 (94%)	23 (6%)	18	37
2	G	753/768 (98%)	695 (92%)	58 (8%)	12	25
2	H	750/768 (98%)	686 (92%)	64 (8%)	10	22
All	All	2287/2374 (96%)	2118 (93%)	169 (7%)	13	27

All (169) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	VAL
1	A	73	GLU
1	A	93	GLN
1	A	102	ILE
1	A	117	THR
1	A	121	GLU
1	A	132	ARG
1	A	151	GLU
1	A	167	ASP
1	A	200	LYS
1	A	211	GLU
1	A	221	THR
1	A	222	LYS
1	A	233	GLN
1	A	243	GLN
1	A	247	LYS
1	A	273	SER
1	A	340	THR
1	A	367	GLN
1	A	379	ASP
1	A	402	GLN
1	A	419	ASN
1	A	433	GLU
1	A	475	GLN

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Mol	Chain	Res	Type
1	B	42	LYS
1	B	71	LYS
1	B	93	GLN
1	B	112	SER
1	B	117	THR
1	B	130	LYS
1	B	131	LYS
1	B	132	ARG
1	B	199	ASP
1	B	211	GLU
1	B	221	THR
1	B	234	LEU
1	B	271	LYS
1	B	273	SER
1	B	330	GLU
1	B	332	GLU
1	B	337	GLU
1	B	340	THR
1	B	344	HIS
1	B	351	ILE
1	B	362	GLU
1	B	367	GLN
1	B	436	LYS
2	G	46	ARG
2	G	90	GLU
2	G	109	LYS
2	G	113	LYS
2	G	123	THR
2	G	145	ILE
2	G	170	ILE
2	G	179	GLN
2	G	231	LEU
2	G	252	SER
2	G	269	SER
2	G	272	GLN
2	G	287	ILE
2	G	293	VAL
2	G	298	CYS
2	G	305	SER
2	G	318	ASP
2	G	321	SER
2	G	346	GLN

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Mol	Chain	Res	Type
2	G	353	LYS
2	G	354	GLU
2	G	369	SER
2	G	377	ASP
2	G	384	ASP
2	G	390	GLN
2	G	411	LEU
2	G	421	SER
2	G	445	CYS
2	G	469	ASP
2	G	491	LYS
2	G	497	GLU
2	G	500	ILE
2	G	513	LEU
2	G	533	LYS
2	G	537	LYS
2	G	586	GLU
2	G	591	LYS
2	G	592	ILE
2	G	597	LEU
2	G	656	LYS
2	G	674	LEU
2	G	675	ILE
2	G	678	THR
2	G	686	LEU
2	G	711	SER
2	G	715	SER
2	G	716	LYS
2	G	744	GLN
2	G	759	ILE
2	G	772	ARG
2	G	779	LYS
2	G	781	ARG
2	G	814	ILE
2	G	821	GLN
2	G	830	MET
2	G	848	SER
2	G	849	THR
2	G	885	GLN
2	H	32	ARG
2	H	46	ARG
2	H	90	GLU

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Mol	Chain	Res	Type
2	H	113	LYS
2	H	123	THR
2	H	133	LYS
2	H	145	ILE
2	H	170	ILE
2	H	188	ILE
2	H	224	ASP
2	H	225	SER
2	H	231	LEU
2	H	252	SER
2	H	266	ARG
2	H	268	MET
2	H	272	GLN
2	H	287	ILE
2	H	298	CYS
2	H	305	SER
2	H	318	ASP
2	H	321	SER
2	H	346	GLN
2	H	350	MET
2	H	353	LYS
2	H	354	GLU
2	H	369	SER
2	H	377	ASP
2	H	384	ASP
2	H	411	LEU
2	H	421	SER
2	H	431	ILE
2	H	434	THR
2	H	445	CYS
2	H	446	LYS
2	H	466	LYS
2	H	467	LYS
2	H	469	ASP
2	H	471	ARG
2	H	497	GLU
2	H	500	ILE
2	H	519	GLU
2	H	571	MET
2	H	592	ILE
2	H	623	ARG
2	H	626	ARG

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Mol	Chain	Res	Type
2	H	644	ARG
2	H	654	ILE
2	H	656	LYS
2	H	675	ILE
2	H	684	GLU
2	H	686	LEU
2	H	711	SER
2	H	715	SER
2	H	716	LYS
2	H	717	MET
2	H	759	ILE
2	H	768	SER
2	H	779	LYS
2	H	781	ARG
2	H	791	THR
2	H	820	SER
2	H	821	GLN
2	H	830	MET
2	H	848	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	224	ASN
1	A	419	ASN
1	A	475	GLN
1	B	41	HIS
1	B	224	ASN
1	B	233	GLN
1	B	344	HIS
1	B	354	HIS
1	B	367	GLN
1	B	402	GLN
2	G	22	HIS
2	G	91	ASN
2	G	120	GLN
2	G	173	ASN
2	G	334	GLN
2	G	390	GLN
2	G	535	HIS
2	G	549	ASN
2	G	559	ASN

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Mol	Chain	Res	Type
2	G	647	ASN
2	G	649	ASN
2	G	685	ASN
2	G	700	GLN
2	G	744	GLN
2	G	780	ASN
2	H	120	GLN
2	H	173	ASN
2	H	244	GLN
2	H	254	GLN
2	H	272	GLN
2	H	316	GLN
2	H	334	GLN
2	H	390	GLN
2	H	442	ASN
2	H	531	ASN
2	H	535	HIS
2	H	663	GLN
2	H	742	GLN
2	H	780	ASN
2	H	818	GLN
2	H	821	GLN
2	H	839	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 51 ligands modelled in this entry, 2 are monoatomic - leaving 49 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	$\# Z > 2$
6	SO4	G	907	-	4,4,4	0.31	0	6,6,6	0.08	0
5	PGE	B	603	-	9,9,9	0.16	0	8,8,8	0.14	0
4	EDO	H	912	-	3,3,3	0.12	0	2,2,2	0.06	0
6	SO4	G	904	-	4,4,4	0.28	0	6,6,6	0.10	0
6	SO4	H	907	-	4,4,4	0.36	0	6,6,6	0.16	0
4	EDO	G	914	-	3,3,3	0.13	0	2,2,2	0.12	0
4	EDO	A	606	-	3,3,3	0.09	0	2,2,2	0.12	0
4	EDO	A	602	-	3,3,3	0.06	0	2,2,2	0.01	0
4	EDO	A	603	-	3,3,3	0.30	0	2,2,2	0.82	0
4	EDO	G	915	-	3,3,3	0.04	0	2,2,2	0.21	0
6	SO4	G	909	-	4,4,4	0.36	0	6,6,6	0.10	0
7	PEG	B	608	-	6,6,6	0.17	0	5,5,5	0.06	0
5	PGE	H	904	-	9,9,9	0.18	0	8,8,8	0.16	0
4	EDO	H	913	-	3,3,3	0.11	0	2,2,2	0.25	0
6	SO4	G	908	-	4,4,4	0.40	0	6,6,6	0.27	0
8	PE5	H	901	-	26,26,26	0.29	0	25,25,25	0.14	0
5	PGE	H	905	-	9,9,9	0.22	0	8,8,8	0.13	0
7	PEG	H	916	-	6,6,6	0.14	0	5,5,5	0.08	0
4	EDO	A	605	-	3,3,3	0.08	0	2,2,2	0.12	0
6	SO4	G	906	-	4,4,4	0.26	0	6,6,6	0.20	0
7	PEG	B	609	-	6,6,6	0.19	0	5,5,5	0.15	0
6	SO4	H	906	-	4,4,4	0.39	0	6,6,6	0.33	0
10	PE4	H	902	-	23,23,23	0.22	0	22,22,22	0.16	0
5	PGE	H	903	-	9,9,9	0.18	0	8,8,8	0.27	0
7	PEG	G	917	-	6,6,6	0.21	0	5,5,5	0.13	0
6	SO4	G	905	-	4,4,4	0.35	0	6,6,6	0.16	0
4	EDO	G	916	-	3,3,3	0.28	0	2,2,2	0.57	0
5	PGE	G	902	-	9,9,9	0.23	0	8,8,8	0.22	0
8	PE5	G	901	-	26,26,26	0.34	0	25,25,25	0.16	0
6	SO4	B	604	-	4,4,4	0.31	0	6,6,6	0.13	0
4	EDO	B	607	-	3,3,3	0.08	0	2,2,2	0.43	0
4	EDO	B	606	-	3,3,3	0.17	0	2,2,2	0.47	0
4	EDO	G	913	-	3,3,3	0.10	0	2,2,2	0.13	0
4	EDO	H	909	-	3,3,3	0.13	0	2,2,2	0.39	0
9	TRS	G	903	-	7,7,7	0.15	0	9,9,9	0.45	0
6	SO4	G	910	-	4,4,4	0.32	0	6,6,6	0.08	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	EDO	A	604	-	3,3,3	0.21	0	2,2,2	0.34	0
4	EDO	G	912	-	3,3,3	0.07	0	2,2,2	0.15	0
4	EDO	G	911	-	3,3,3	0.26	0	2,2,2	0.36	0
4	EDO	H	911	-	3,3,3	0.09	0	2,2,2	0.24	0
6	SO4	H	908	-	4,4,4	0.31	0	6,6,6	0.10	0
7	PEG	H	915	-	6,6,6	0.13	0	5,5,5	0.09	0
7	PEG	G	918	-	6,6,6	0.16	0	5,5,5	0.06	0
4	EDO	H	910	-	3,3,3	0.04	0	2,2,2	0.23	0
7	PEG	H	914	-	6,6,6	0.10	0	5,5,5	0.13	0
7	PEG	H	917	-	6,6,6	0.30	0	5,5,5	0.23	0
7	PEG	H	918	-	6,6,6	0.16	0	5,5,5	0.04	0
5	PGE	B	602	-	9,9,9	0.20	0	8,8,8	0.12	0
4	EDO	B	605	-	3,3,3	0.24	0	2,2,2	0.33	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	PGE	B	603	-	-	7/7/7/7	-
4	EDO	H	912	-	-	1/1/1/1	-
4	EDO	G	914	-	-	1/1/1/1	-
4	EDO	A	606	-	-	0/1/1/1	-
4	EDO	A	602	-	-	1/1/1/1	-
4	EDO	A	603	-	-	0/1/1/1	-
4	EDO	G	915	-	-	0/1/1/1	-
7	PEG	B	608	-	-	2/4/4/4	-
5	PGE	H	904	-	-	5/7/7/7	-
4	EDO	H	913	-	-	0/1/1/1	-
8	PE5	H	901	-	-	14/24/24/24	-
5	PGE	H	905	-	-	3/7/7/7	-
7	PEG	H	916	-	-	2/4/4/4	-
4	EDO	A	605	-	-	1/1/1/1	-
7	PEG	B	609	-	-	2/4/4/4	-
10	PE4	H	902	-	-	14/21/21/21	-
5	PGE	H	903	-	-	5/7/7/7	-
7	PEG	G	917	-	-	3/4/4/4	-
4	EDO	G	916	-	-	1/1/1/1	-
5	PGE	G	902	-	-	5/7/7/7	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	PE5	G	901	-	-	15/24/24/24	-
4	EDO	B	607	-	-	1/1/1/1	-
4	EDO	B	606	-	-	1/1/1/1	-
4	EDO	G	913	-	-	1/1/1/1	-
4	EDO	H	909	-	-	1/1/1/1	-
9	TRS	G	903	-	-	0/9/9/9	-
4	EDO	A	604	-	-	0/1/1/1	-
4	EDO	G	912	-	-	0/1/1/1	-
4	EDO	G	911	-	-	1/1/1/1	-
4	EDO	H	911	-	-	1/1/1/1	-
7	PEG	H	915	-	-	1/4/4/4	-
7	PEG	G	918	-	-	0/4/4/4	-
4	EDO	H	910	-	-	1/1/1/1	-
7	PEG	H	914	-	-	2/4/4/4	-
7	PEG	H	917	-	-	2/4/4/4	-
7	PEG	H	918	-	-	4/4/4/4	-
5	PGE	B	602	-	-	5/7/7/7	-
4	EDO	B	605	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (104) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	H	902	PE4	C3-C4-O3-C5
5	G	902	PGE	C3-C4-O3-C5
8	G	901	PE5	O3-C5-C6-O4
8	H	901	PE5	O2-C3-C4-O3
5	G	902	PGE	O2-C3-C4-O3
8	G	901	PE5	O6-C10-C9-O5
10	H	902	PE4	O6-C10-C9-O5
7	G	917	PEG	O1-C1-C2-O2
5	H	904	PGE	O2-C3-C4-O3
8	G	901	PE5	O6-C11-C12-O7
8	G	901	PE5	O1-C1-C2-O2
7	H	917	PEG	O2-C3-C4-O4
8	H	901	PE5	O3-C5-C6-O4
8	G	901	PE5	O2-C3-C4-O3
5	B	603	PGE	O2-C3-C4-O3

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Mol	Chain	Res	Type	Atoms
5	H	903	PGE	O2-C3-C4-O3
10	H	902	PE4	O4-C7-C8-O5
8	G	901	PE5	O4-C7-C8-O5
5	B	603	PGE	O1-C1-C2-O2
5	G	902	PGE	O3-C5-C6-O4
7	H	914	PEG	O1-C1-C2-O2
8	G	901	PE5	O8-C15-C16-O52
5	B	602	PGE	O1-C1-C2-O2
5	B	603	PGE	O3-C5-C6-O4
4	A	602	EDO	O1-C1-C2-O2
4	G	916	EDO	O1-C1-C2-O2
4	H	909	EDO	O1-C1-C2-O2
4	H	912	EDO	O1-C1-C2-O2
5	H	903	PGE	O3-C5-C6-O4
5	G	902	PGE	C4-C3-O2-C2
5	H	903	PGE	C3-C4-O3-C5
10	H	902	PE4	O7-C13-C14-O8
8	G	901	PE5	O7-C13-C14-O8
7	H	915	PEG	O2-C3-C4-O4
8	H	901	PE5	O8-C15-C16-O52
4	G	913	EDO	O1-C1-C2-O2
5	H	905	PGE	O3-C5-C6-O4
8	G	901	PE5	C9-C10-O6-C11
8	G	901	PE5	C48-C50-O1-C1
10	H	902	PE4	O1-C1-C2-O2
8	H	901	PE5	C48-C50-O1-C1
4	B	607	EDO	O1-C1-C2-O2
4	H	910	EDO	O1-C1-C2-O2
7	H	918	PEG	O1-C1-C2-O2
10	H	902	PE4	O6-C11-C12-O7
7	B	609	PEG	C4-C3-O2-C2
8	G	901	PE5	C13-C14-O8-C15
10	H	902	PE4	C12-C11-O6-C10
10	H	902	PE4	C8-C7-O4-C6
5	H	904	PGE	C6-C5-O3-C4
7	B	609	PEG	C1-C2-O2-C3
8	H	901	PE5	C6-C5-O3-C4
7	H	918	PEG	C1-C2-O2-C3
5	B	603	PGE	C1-C2-O2-C3
7	H	916	PEG	C1-C2-O2-C3
8	H	901	PE5	C11-C12-O7-C13
7	B	608	PEG	C4-C3-O2-C2

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Mol	Chain	Res	Type	Atoms
8	H	901	PE5	C9-C10-O6-C11
10	H	902	PE4	C13-C14-O8-C15
8	G	901	PE5	C4-C3-O2-C2
5	G	902	PGE	C6-C5-O3-C4
5	H	904	PGE	C3-C4-O3-C5
7	H	918	PEG	C4-C3-O2-C2
8	H	901	PE5	C13-C14-O8-C15
8	G	901	PE5	C12-C11-O6-C10
5	H	905	PGE	C4-C3-O2-C2
5	B	603	PGE	C6-C5-O3-C4
7	H	916	PEG	C4-C3-O2-C2
5	H	904	PGE	O1-C1-C2-O2
5	B	602	PGE	C1-C2-O2-C3
5	B	602	PGE	C6-C5-O3-C4
8	G	901	PE5	C7-C8-O5-C9
7	G	917	PEG	C4-C3-O2-C2
7	G	917	PEG	C1-C2-O2-C3
8	H	901	PE5	C2-C1-O1-C50
5	B	602	PGE	C3-C4-O3-C5
8	G	901	PE5	C10-C9-O5-C8
10	H	902	PE4	O3-C5-C6-O4
8	H	901	PE5	C16-C15-O8-C14
10	H	902	PE4	C16-C15-O8-C14
5	B	603	PGE	C4-C3-O2-C2
8	H	901	PE5	O6-C10-C9-O5
7	H	917	PEG	C4-C3-O2-C2
5	B	602	PGE	C4-C3-O2-C2
4	A	605	EDO	O1-C1-C2-O2
4	G	914	EDO	O1-C1-C2-O2
7	B	608	PEG	C1-C2-O2-C3
5	H	904	PGE	O3-C5-C6-O4
8	H	901	PE5	O1-C1-C2-O2
5	H	903	PGE	C4-C3-O2-C2
7	H	914	PEG	C4-C3-O2-C2
4	H	911	EDO	O1-C1-C2-O2
5	B	603	PGE	C3-C4-O3-C5
10	H	902	PE4	O2-C3-C4-O3
10	H	902	PE4	C4-C3-O2-C2
4	B	606	EDO	O1-C1-C2-O2
4	G	911	EDO	O1-C1-C2-O2
5	H	903	PGE	O1-C1-C2-O2
7	H	918	PEG	O2-C3-C4-O4

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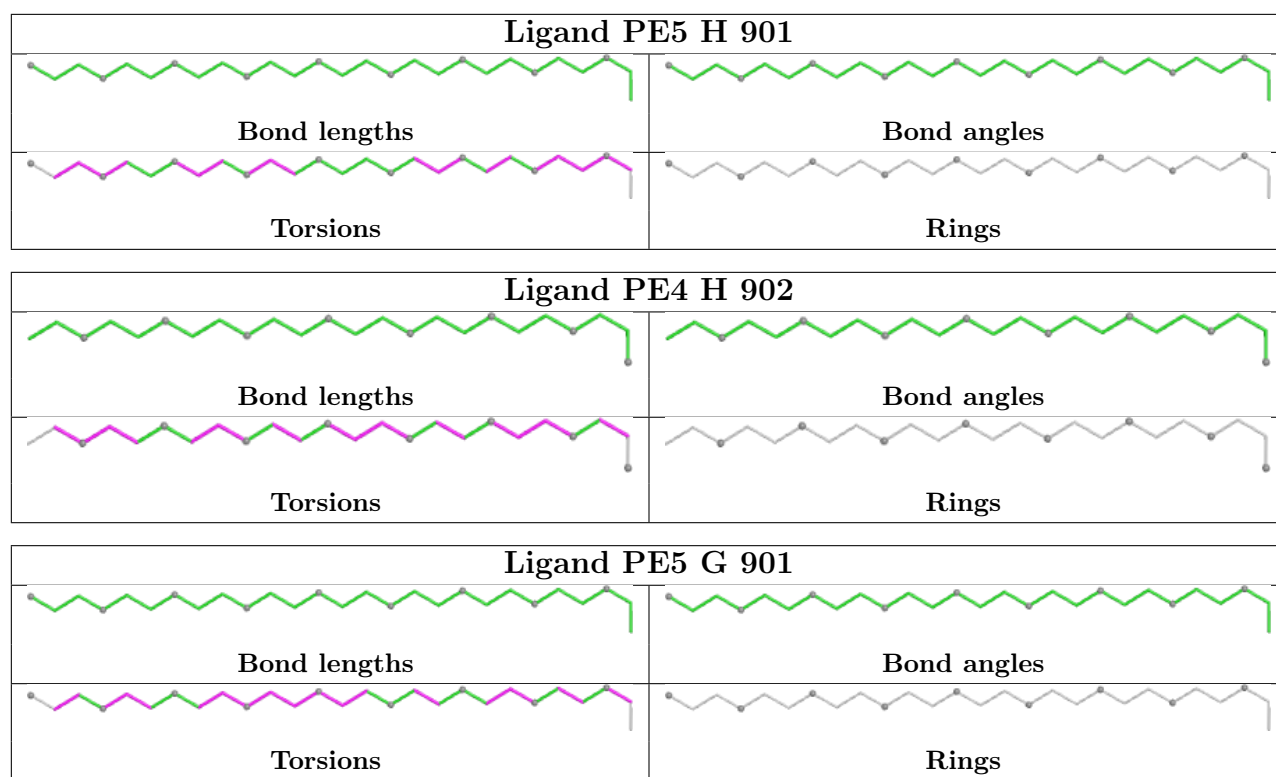
Mol	Chain	Res	Type	Atoms
8	H	901	PE5	O6-C11-C12-O7
5	H	905	PGE	C6-C5-O3-C4
8	H	901	PE5	C1-C2-O2-C3
10	H	902	PE4	C7-C8-O5-C9
4	B	605	EDO	O1-C1-C2-O2

There are no ring outliers.

17 monomers are involved in 33 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	G	907	SO4	1	0
5	B	603	PGE	1	0
4	A	602	EDO	1	0
4	A	603	EDO	2	0
4	G	915	EDO	1	0
8	H	901	PE5	6	0
5	H	905	PGE	1	0
6	G	906	SO4	1	0
6	H	906	SO4	1	0
10	H	902	PE4	2	0
5	H	903	PGE	1	0
5	G	902	PGE	5	0
8	G	901	PE5	1	0
9	G	903	TRS	1	0
4	A	604	EDO	1	0
7	H	914	PEG	2	0
7	H	917	PEG	5	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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	461/492 (93%)	-0.16	1 (0%) 91 89	26, 75, 149, 188	1 (0%)
1	B	462/492 (93%)	-0.19	0 100 100	39, 72, 120, 167	1 (0%)
2	G	863/884 (97%)	-0.31	0 100 100	28, 61, 107, 150	4 (0%)
2	H	862/884 (97%)	-0.18	8 (0%) 81 78	25, 64, 122, 167	2 (0%)
All	All	2648/2752 (96%)	-0.22	9 (0%) 90 87	25, 65, 127, 188	8 (0%)

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	464	ALA	3.2
2	H	260	THR	2.8
2	H	840[A]	PHE	2.7
2	H	276	ILE	2.4
2	H	270	GLY	2.3
2	H	273	ALA	2.3
2	H	710	TYR	2.2
1	A	111	ALA	2.1
2	H	284	TYR	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 oligosaccharides 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	EDO	G	912	4/4	0.70	0.31	72,78,81,83	4
4	EDO	G	913	4/4	0.71	0.10	90,96,103,106	0
4	EDO	G	914	4/4	0.71	0.17	101,104,110,113	0
4	EDO	H	913	4/4	0.71	0.19	78,81,82,85	4
4	EDO	B	607	4/4	0.75	0.23	69,72,76,78	4
4	EDO	H	910	4/4	0.76	0.13	94,98,102,104	0
4	EDO	G	915	4/4	0.76	0.28	57,60,63,65	4
10	PE4	H	902	24/24	0.77	0.22	84,109,117,122	24
6	SO4	G	909	5/5	0.79	0.12	78,81,86,89	5
6	SO4	G	906	5/5	0.79	0.13	64,65,74,75	5
5	PGE	H	903	10/10	0.82	0.14	64,73,81,85	10
4	EDO	A	604	4/4	0.82	0.16	71,84,84,92	0
7	PEG	H	916	7/7	0.83	0.15	89,101,106,106	7
4	EDO	B	605	4/4	0.84	0.18	79,89,90,92	0
4	EDO	B	606	4/4	0.86	0.12	88,90,96,96	0
7	PEG	B	609	7/7	0.86	0.20	60,69,80,81	7
7	PEG	G	918	7/7	0.86	0.15	62,79,88,89	7
5	PGE	H	904	10/10	0.86	0.13	67,78,96,99	10
7	PEG	H	917	7/7	0.86	0.14	66,71,78,78	7
4	EDO	H	909	4/4	0.86	0.12	75,82,91,91	0
4	EDO	H	912	4/4	0.87	0.13	98,103,111,115	0
4	EDO	G	911	4/4	0.87	0.18	64,79,85,91	0
5	PGE	B	602	10/10	0.87	0.14	67,76,90,93	10
4	EDO	H	911	4/4	0.87	0.09	81,88,93,94	0
4	EDO	G	916	4/4	0.88	0.12	64,69,71,75	0
6	SO4	G	904	5/5	0.88	0.10	77,78,83,88	5
5	PGE	G	902	10/10	0.88	0.18	65,69,88,88	10
4	EDO	A	602	4/4	0.88	0.10	68,71,73,75	0
6	SO4	G	910	5/5	0.88	0.11	87,87,90,91	5
8	PE5	G	901	27/27	0.89	0.31	85,106,117,126	27
7	PEG	H	918	7/7	0.90	0.11	71,78,87,95	7
4	EDO	A	603	4/4	0.90	0.22	64,66,67,68	0
8	PE5	H	901	27/27	0.90	0.32	70,98,130,142	27
4	EDO	A	606	4/4	0.90	0.10	96,106,110,114	0
5	PGE	B	603	10/10	0.91	0.20	92,98,103,105	10
4	EDO	A	605	4/4	0.91	0.10	62,72,73,76	0
6	SO4	G	907	5/5	0.91	0.06	76,78,85,87	5

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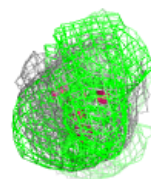
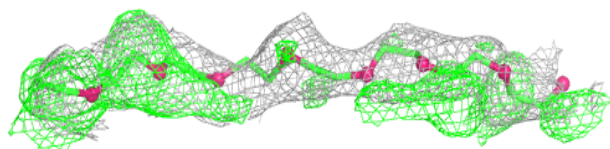
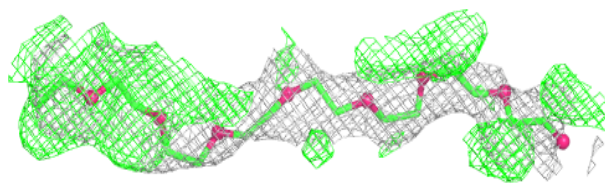
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	PEG	H	915	7/7	0.91	0.17	76,77,81,82	7
6	SO4	B	604	5/5	0.91	0.10	63,65,73,76	5
7	PEG	H	914	7/7	0.92	0.12	77,89,90,91	0
5	PGE	H	905	10/10	0.92	0.11	83,89,102,103	0
7	PEG	G	917	7/7	0.92	0.12	67,83,95,102	0
7	PEG	B	608	7/7	0.92	0.13	65,74,81,82	7
6	SO4	H	908	5/5	0.93	0.10	66,69,74,76	5
6	SO4	H	907	5/5	0.94	0.08	63,65,72,72	5
6	SO4	G	905	5/5	0.95	0.07	66,68,72,74	5
9	TRS	G	903	8/8	0.95	0.11	51,62,66,74	0
6	SO4	H	906	5/5	0.95	0.06	66,68,80,80	0
3	CA	B	601	1/1	0.96	0.07	60,60,60,60	0
6	SO4	G	908	5/5	0.96	0.07	47,48,54,57	0
3	CA	A	601	1/1	0.97	0.09	57,57,57,57	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

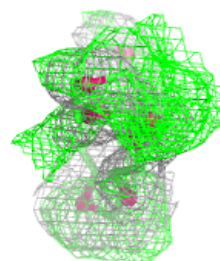
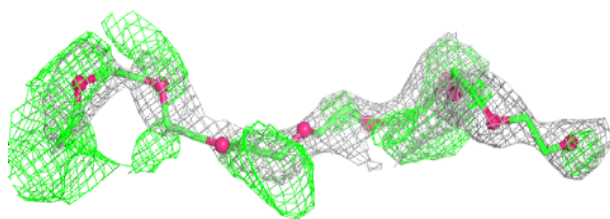
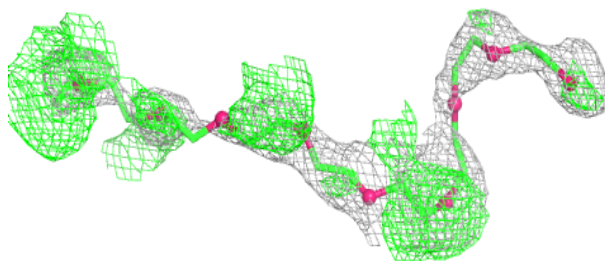
Electron density around PE4 H 902:

2mF_o-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

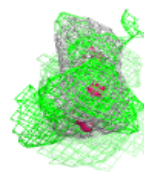
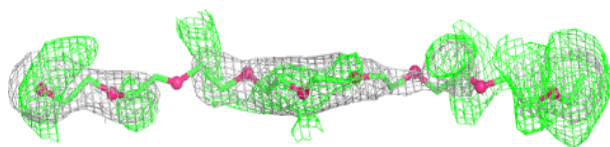
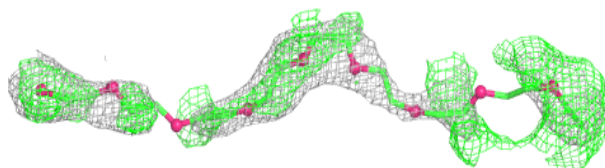


Electron density around PE5 G 901:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around PE5 H 901:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.