



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 09:47 PM UTC

PDB ID : 4ZUL / pdb_00004zul
Title : Structure ALDH7A1 complexed with alpha-aminoadipate
Authors : Luo, M.; Tanner, J.J.
Deposited on : 2015-05-16
Resolution : 1.76 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
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

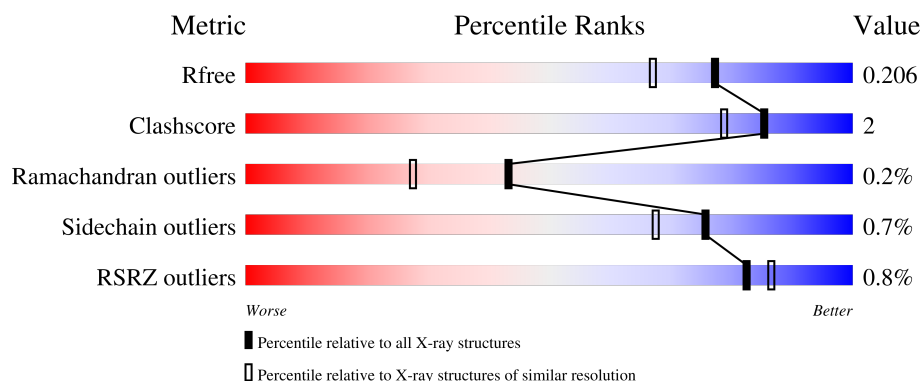
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.76 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	3183 (1.76-1.76)
Clashscore	190562	3299 (1.76-1.76)
Ramachandran outliers	187476	3274 (1.76-1.76)
Sidechain outliers	187428	3274 (1.76-1.76)
RSRZ outliers	180081	3183 (1.76-1.76)

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	513	% 95% ..
1	B	513	% 93% 6% .
1	C	513	% 94% 5% .
1	D	513	2% 93% 6% .
1	E	513	% 91% 8% .

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Mol	Chain	Length	Quality of chain
1	F	513	% 93% 7%
1	G	513	% 91% 8%
1	H	513	% 92% 7%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 32645 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 Alpha-aminoadipic semialdehyde dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	509	Total	C	N	O	S	0	3	0
			3834	2440	664	712	18			
1	B	509	Total	C	N	O	S	0	4	0
			3815	2431	665	701	18			
1	C	508	Total	C	N	O	S	0	2	0
			3824	2436	663	706	19			
1	D	509	Total	C	N	O	S	0	1	0
			3795	2416	656	705	18			
1	E	508	Total	C	N	O	S	0	1	0
			3821	2435	665	703	18			
1	F	509	Total	C	N	O	S	0	2	0
			3831	2438	666	709	18			
1	G	509	Total	C	N	O	S	0	2	0
			3814	2428	662	706	18			
1	H	509	Total	C	N	O	S	0	2	0
			3828	2435	662	713	18			

There are 16 discrepancies between the modelled and reference sequences:

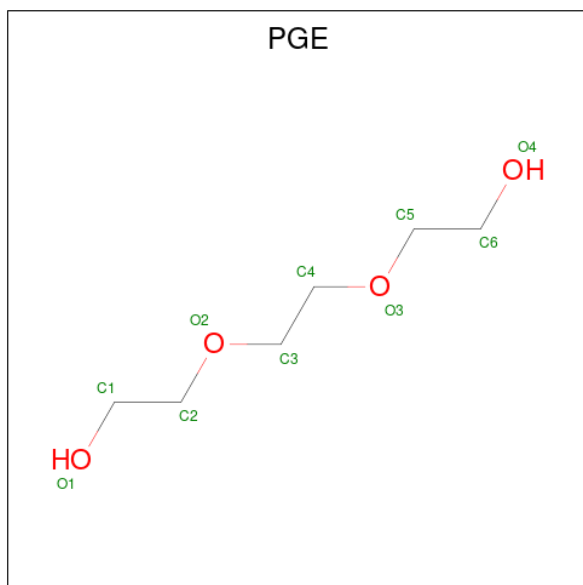
Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP P49419
A	0	HIS	-	expression tag	UNP P49419
B	-1	GLY	-	expression tag	UNP P49419
B	0	HIS	-	expression tag	UNP P49419
C	-1	GLY	-	expression tag	UNP P49419
C	0	HIS	-	expression tag	UNP P49419
D	-1	GLY	-	expression tag	UNP P49419
D	0	HIS	-	expression tag	UNP P49419
E	-1	GLY	-	expression tag	UNP P49419
E	0	HIS	-	expression tag	UNP P49419
F	-1	GLY	-	expression tag	UNP P49419
F	0	HIS	-	expression tag	UNP P49419
G	-1	GLY	-	expression tag	UNP P49419

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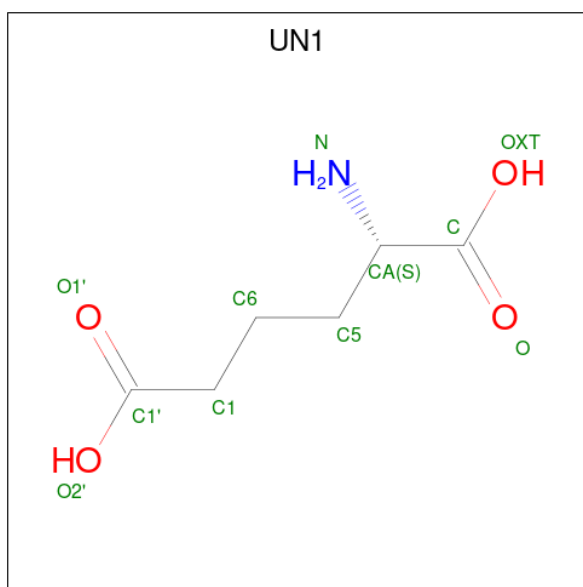
Chain	Residue	Modelled	Actual	Comment	Reference
G	0	HIS	-	expression tag	UNP P49419
H	-1	GLY	-	expression tag	UNP P49419
H	0	HIS	-	expression tag	UNP P49419

- Molecule 2 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: $C_6H_{14}O_4$).



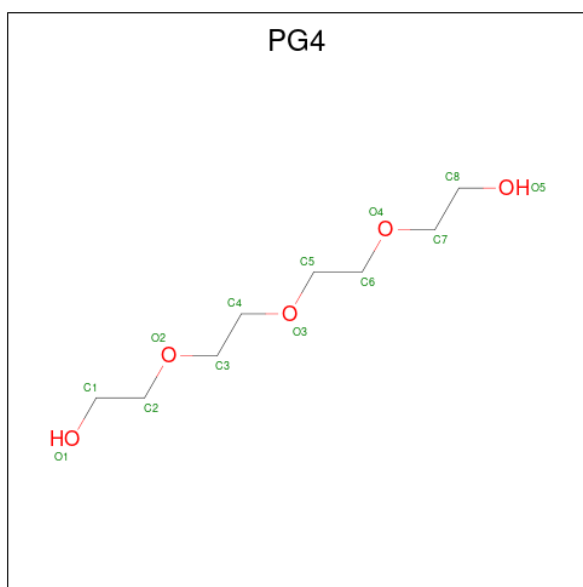
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			10	6	4		
2	B	1	Total	C	O	0	0
			10	6	4		
2	C	1	Total	C	O	0	0
			10	6	4		
2	D	1	Total	C	O	0	0
			10	6	4		
2	F	1	Total	C	O	0	0
			10	6	4		
2	G	1	Total	C	O	0	0
			10	6	4		
2	H	1	Total	C	O	0	0
			10	6	4		

- Molecule 3 is 2-AMINOHEXANEDIOIC ACID (CCD ID: UN1) (formula: $C_6H_{11}NO_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			11	6	1	4		
3	B	1	Total	C	N	O	0	0
			11	6	1	4		
3	C	1	Total	C	N	O	0	0
			11	6	1	4		
3	D	1	Total	C	N	O	0	0
			11	6	1	4		
3	E	1	Total	C	N	O	0	0
			11	6	1	4		
3	F	1	Total	C	N	O	0	0
			11	6	1	4		
3	G	1	Total	C	N	O	0	0
			11	6	1	4		
3	H	1	Total	C	N	O	0	0
			11	6	1	4		

- Molecule 4 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: C₈H₁₈O₅).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	E	1	Total	C	O	0	0
			13	8	5		
4	H	1	Total	C	O	0	0
			13	8	5		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	225	Total	O	0	0
			225	225		
5	B	249	Total	O	0	0
			249	249		
5	C	252	Total	O	0	0
			252	252		
5	D	214	Total	O	0	0
			214	214		
5	E	249	Total	O	0	0
			249	249		
5	F	243	Total	O	0	0
			243	243		
5	G	239	Total	O	0	0
			239	239		
5	H	228	Total	O	0	0
			228	228		

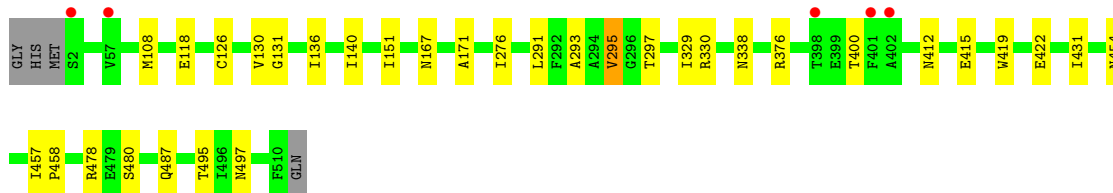
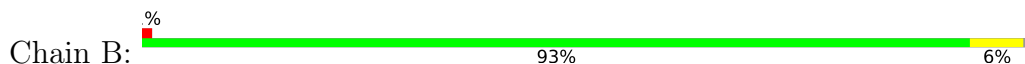
3 Residue-property plots [i](#)

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.

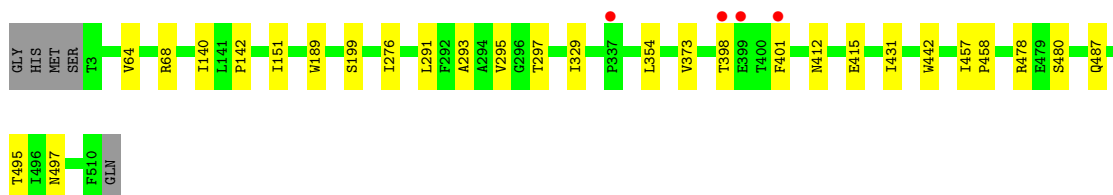
- Molecule 1: Alpha-aminoadipic semialdehyde dehydrogenase



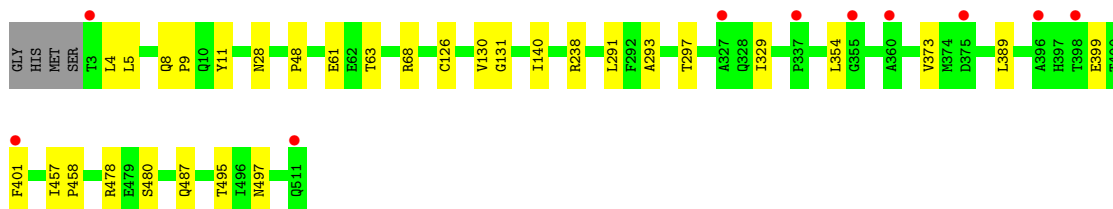
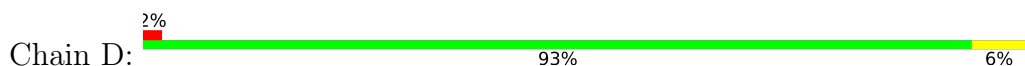
- Molecule 1: Alpha-aminoadipic semialdehyde dehydrogenase



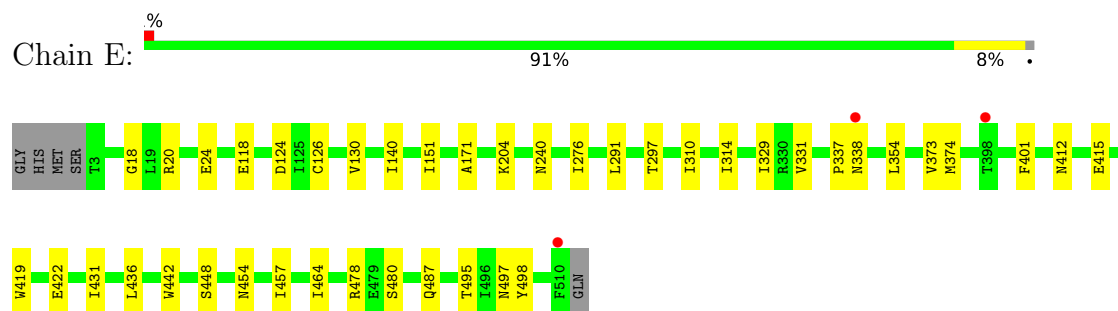
- Molecule 1: Alpha-aminoadipic semialdehyde dehydrogenase



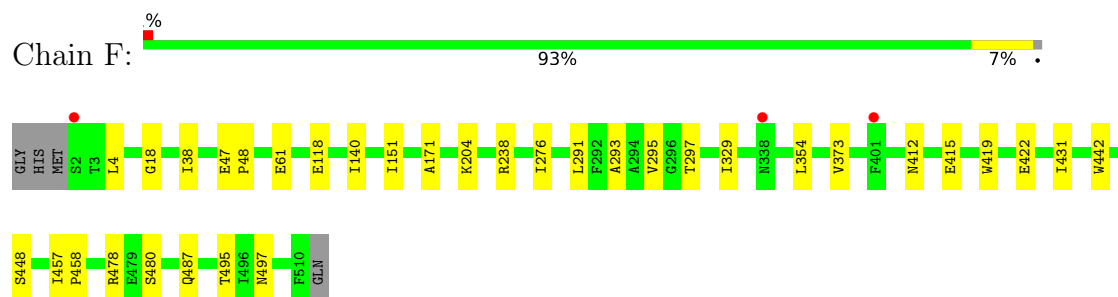
- Molecule 1: Alpha-aminoadipic semialdehyde dehydrogenase



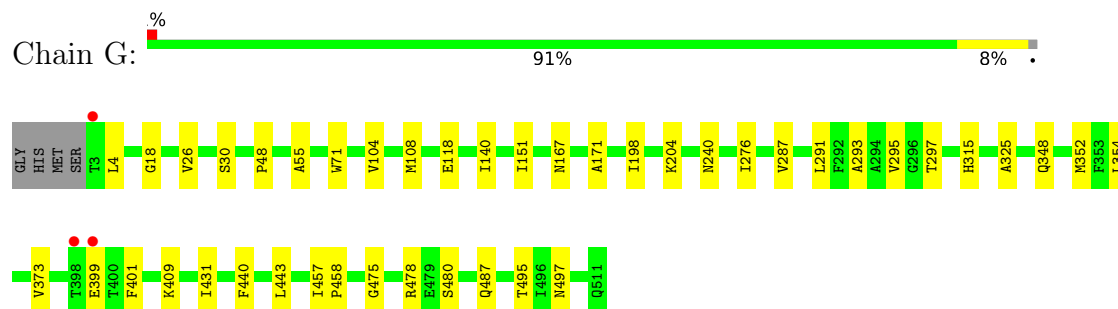
- Molecule 1: Alpha-aminoadipic semialdehyde dehydrogenase



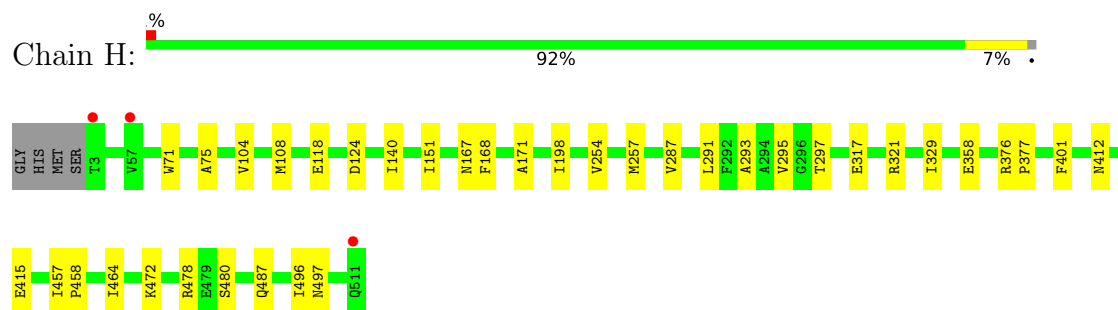
- Molecule 1: Alpha-aminoadipic semialdehyde dehydrogenase



- Molecule 1: Alpha-aminoadipic semialdehyde dehydrogenase



- Molecule 1: Alpha-aminoadipic semialdehyde dehydrogenase



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	154.43Å 162.53Å 158.68Å 90.00° 95.04° 90.00°	Depositor
Resolution (Å)	41.79 – 1.76 41.79 – 1.76	Depositor EDS
% Data completeness (in resolution range)	99.3 (41.79-1.76) 99.3 (41.79-1.76)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.20 (at 1.76Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.168 , 0.206 0.169 , 0.206	Depositor DCC
R_{free} test set	19260 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	20.3	Xtriage
Anisotropy	0.515	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 45.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	32645	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.38% 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: PG4, UN1, 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	0.44	0/3924	0.75	2/5331 (0.0%)
1	B	0.44	0/3905	0.74	0/5307
1	C	0.45	0/3910	0.74	0/5310
1	D	0.41	0/3878	0.73	0/5275
1	E	0.45	0/3904	0.76	0/5300
1	F	0.44	0/3918	0.75	0/5320
1	G	0.44	0/3897	0.73	3/5296 (0.1%)
1	H	0.43	0/3914	0.77	3/5319 (0.1%)
All	All	0.44	0/31250	0.75	8/42458 (0.0%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	141	LEU	CA-C-N	-5.44	113.98	120.13
1	A	141	LEU	C-N-CA	-5.44	113.98	120.13
1	H	287	VAL	CA-C-N	-5.37	114.14	119.56
1	H	287	VAL	C-N-CA	-5.37	114.14	119.56
1	G	287	VAL	CA-C-N	-5.29	114.22	119.56
1	G	287	VAL	C-N-CA	-5.29	114.22	119.56
1	G	475	GLY	N-CA-C	5.15	119.81	113.79
1	H	472	LYS	CB-CA-C	-5.06	110.76	116.63

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	3834	0	3800	17	0
1	B	3815	0	3774	22	0
1	C	3824	0	3797	18	0
1	D	3795	0	3728	18	0
1	E	3821	0	3807	24	0
1	F	3831	0	3802	19	0
1	G	3814	0	3766	24	0
1	H	3828	0	3784	20	0
2	A	10	0	14	4	0
2	B	10	0	14	0	0
2	C	10	0	14	0	0
2	D	10	0	14	1	0
2	F	10	0	14	0	0
2	G	10	0	14	3	0
2	H	10	0	14	0	0
3	A	11	0	4	0	0
3	B	11	0	4	0	0
3	C	11	0	4	0	0
3	D	11	0	4	0	0
3	E	11	0	4	0	0
3	F	11	0	4	0	0
3	G	11	0	4	0	0
3	H	11	0	4	1	0
4	E	13	0	18	1	0
4	H	13	0	18	0	0
5	A	225	0	0	2	0
5	B	249	0	0	0	0
5	C	252	0	0	1	0
5	D	214	0	0	1	0
5	E	249	0	0	0	0
5	F	243	0	0	0	0
5	G	239	0	0	0	0
5	H	228	0	0	0	0
All	All	32645	0	30424	136	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 2.

All (136) 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:A:240:ASN:HD21	2:A:601:PGE:H1	1.51	0.75
1:H:376[B]:ARG:HH21	1:H:376[B]:ARG:HG3	1.53	0.74
1:G:478:ARG:O	1:G:487:GLN:NE2	2.21	0.71
1:C:478:ARG:O	1:C:487:GLN:NE2	2.23	0.71
1:B:376[B]:ARG:HH21	1:B:376[B]:ARG:HG3	1.55	0.71
1:F:291:LEU:HD11	1:F:329:ILE:HD11	1.72	0.70
1:A:478:ARG:O	1:A:487:GLN:NE2	2.25	0.69
1:D:478:ARG:O	1:D:487:GLN:NE2	2.27	0.66
1:E:18:GLY:O	1:E:204:LYS:NZ	2.28	0.66
1:E:20:ARG:NH2	1:E:24:GLU:OE1	2.25	0.66
1:F:118:GLU:HG3	1:F:171:ALA:HB2	1.78	0.66
1:C:354:LEU:HD21	1:C:373:VAL:HG23	1.78	0.65
1:H:118:GLU:HG3	1:H:171:ALA:HB2	1.78	0.64
1:B:478:ARG:O	1:B:487:GLN:NE2	2.30	0.63
1:H:317:GLU:OE2	1:H:321:ARG:NH2	2.33	0.62
1:A:68:ARG:HH22	2:A:601:PGE:H12	1.63	0.62
1:E:478:ARG:O	1:E:487:GLN:NE2	2.32	0.62
1:H:376[B]:ARG:NH2	1:H:377:PRO:O	2.34	0.61
1:F:478:ARG:O	1:F:487:GLN:NE2	2.34	0.61
1:D:291:LEU:HD11	1:D:329:ILE:HD11	1.82	0.60
1:G:118:GLU:HG3	1:G:171:ALA:HB2	1.84	0.60
1:C:412:ASN:ND2	5:C:703:HOH:O	2.36	0.57
1:A:264:ARG:NH2	5:A:703:HOH:O	2.37	0.57
5:A:910:HOH:O	1:F:38:ILE:HD11	2.05	0.56
1:A:151:ILE:HB	1:D:140:ILE:HD11	1.88	0.56
1:B:291:LEU:HD11	1:B:329:ILE:HD11	1.86	0.56
1:H:108:MET:HE3	1:H:167:ASN:HA	1.87	0.56
1:A:293:ALA:HB2	1:A:458:PRO:HB3	1.88	0.55
1:B:293:ALA:HB2	1:B:458:PRO:HB3	1.89	0.55
1:H:478:ARG:O	1:H:487:GLN:NE2	2.36	0.55
1:F:354:LEU:HD21	1:F:373:VAL:HG23	1.88	0.54
1:G:348:GLN:O	1:G:352:MET:HG3	2.08	0.53
1:A:457:ILE:HD11	1:B:495:THR:HB	1.90	0.53
1:F:293:ALA:HB2	1:F:458:PRO:HB3	1.89	0.53
1:A:68:ARG:NH2	2:A:601:PGE:H12	2.23	0.53
1:C:457:ILE:HG23	1:D:497:ASN:HB2	1.91	0.53
1:H:104:VAL:HA	1:H:198:ILE:HD11	1.91	0.53
1:D:354:LEU:HD21	1:D:373:VAL:HG23	1.90	0.53
1:C:495:THR:HB	1:D:457:ILE:HD11	1.90	0.52
1:E:140:ILE:HD11	1:H:151:ILE:HB	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:495:THR:HB	1:F:457:ILE:HD11	1.91	0.52
1:E:331:VAL:HG21	1:E:374:MET:HE1	1.92	0.52
1:A:431:ILE:HG23	1:A:442:TRP:CE2	2.45	0.52
1:B:412:ASN:O	1:B:415:GLU:HG2	2.11	0.51
1:G:293:ALA:HB2	1:G:458:PRO:HB3	1.92	0.51
1:H:293:ALA:HB2	1:H:458:PRO:HB3	1.92	0.50
1:E:151:ILE:HB	1:H:140:ILE:HD11	1.93	0.50
1:B:136:ILE:O	1:C:142:PRO:HD3	2.12	0.50
1:B:118:GLU:HG3	1:B:171:ALA:HB2	1.93	0.50
1:E:457:ILE:HD11	1:F:495:THR:HB	1.93	0.50
1:B:376[B]:ARG:HH21	1:B:376[B]:ARG:CG	2.23	0.50
1:G:18:GLY:O	1:G:204:LYS:NZ	2.40	0.50
1:E:291:LEU:HD11	1:E:329:ILE:HD11	1.93	0.49
1:E:457:ILE:HG23	1:F:497:ASN:HB2	1.93	0.49
1:E:354:LEU:HD21	1:E:373:VAL:HG23	1.93	0.49
1:D:61:GLU:OE2	1:D:238:ARG:NH1	2.43	0.49
1:D:68:ARG:CZ	2:D:601:PGE:H2	2.42	0.49
1:F:61:GLU:OE1	1:F:238:ARG:NH2	2.37	0.49
1:C:64:VAL:O	1:C:68:ARG:HG2	2.13	0.49
1:E:412:ASN:O	1:E:415:GLU:HG2	2.12	0.49
1:G:108:MET:HE3	1:G:167:ASN:HA	1.94	0.49
1:G:240:ASN:HD21	2:G:601:PGE:H52	1.78	0.48
1:A:495:THR:HB	1:B:457:ILE:HD11	1.96	0.48
1:G:457:ILE:HG23	1:H:497:ASN:HB2	1.94	0.48
1:D:293:ALA:HB2	1:D:458:PRO:HB3	1.95	0.48
1:C:457:ILE:HD11	1:D:495:THR:HB	1.96	0.48
1:C:293:ALA:HB2	1:C:458:PRO:HB3	1.94	0.48
1:E:454:ASN:HB3	1:E:457:ILE:HG13	1.96	0.48
1:G:276:ILE:HB	1:G:431:ILE:HG22	1.96	0.48
1:F:276:ILE:HB	1:F:431:ILE:HG22	1.95	0.47
1:F:419:TRP:O	1:F:422:GLU:HG2	2.14	0.47
1:A:291:LEU:O	1:A:295:VAL:HG22	2.15	0.47
1:B:108:MET:HE3	1:B:167:ASN:HA	1.97	0.47
1:E:310:ILE:HG22	1:E:314:ILE:HG13	1.97	0.47
1:G:4:LEU:HD23	1:G:48:PRO:HB2	1.97	0.47
1:B:151:ILE:HB	1:C:140:ILE:HD11	1.95	0.47
1:G:291:LEU:HD22	1:G:325:ALA:HB1	1.97	0.47
1:C:291:LEU:O	1:C:295:VAL:HG22	2.15	0.46
1:B:330:ARG:HD3	1:B:338:ASN:O	2.15	0.46
1:H:254:VAL:HA	1:H:257:MET:HE3	1.98	0.45
1:A:240:ASN:HD21	2:A:601:PGE:C1	2.24	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4:LEU:HD23	1:D:48:PRO:HB2	1.98	0.45
1:B:276:ILE:HB	1:B:431:ILE:HG22	1.99	0.45
1:F:140:ILE:HD11	1:G:151:ILE:HB	1.99	0.45
1:G:71:TRP:CE3	2:G:601:PGE:H2	2.52	0.45
1:G:354:LEU:HD21	1:G:373:VAL:HG23	1.98	0.45
1:A:497:ASN:HB2	1:B:457:ILE:HG23	1.99	0.45
1:A:291:LEU:HD22	1:A:325:ALA:HB1	1.99	0.45
1:F:18:GLY:O	1:F:204:LYS:NZ	2.47	0.44
1:G:291:LEU:O	1:G:295:VAL:HG22	2.17	0.44
1:G:443:LEU:HD11	1:H:496:ILE:HD11	1.98	0.44
1:H:168:PHE:CE1	3:H:603:UN1:H6C2	2.52	0.44
1:D:28:ASN:HB3	1:D:63:THR:HG23	2.00	0.44
1:D:126:CYS:O	1:D:130:VAL:HG23	2.17	0.44
1:F:412:ASN:O	1:F:415:GLU:HG2	2.18	0.44
1:A:457:ILE:HG23	1:B:497:ASN:HB2	1.99	0.44
1:E:126:CYS:O	1:E:130:VAL:HG23	2.18	0.44
1:G:495:THR:HB	1:H:457:ILE:HD11	1.99	0.44
1:A:126:CYS:O	1:A:130:VAL:HG23	2.18	0.44
1:G:104:VAL:HA	1:G:198:ILE:HD11	2.00	0.44
1:E:118:GLU:HG3	1:E:171:ALA:HB2	2.00	0.43
1:B:291:LEU:O	1:B:295:VAL:HG22	2.18	0.43
1:E:497:ASN:HB2	1:F:457:ILE:HG23	2.00	0.43
1:H:124:ASP:HB3	1:H:464:ILE:HG12	1.99	0.43
1:F:442:TRP:CH2	1:F:448:SER:HB2	2.54	0.43
1:E:419:TRP:O	1:E:422:GLU:HG2	2.19	0.43
1:B:131:GLY:HA3	1:D:131:GLY:HA3	2.01	0.42
1:E:442:TRP:CH2	1:E:448:SER:HB2	2.54	0.42
1:C:497:ASN:HB2	1:D:457:ILE:HG23	2.00	0.42
1:D:5:LEU:HD22	1:D:11:TYR:CE2	2.55	0.42
1:C:291:LEU:HD11	1:C:329:ILE:HD11	2.00	0.42
1:B:126:CYS:O	1:B:130:VAL:HG23	2.20	0.42
1:F:151:ILE:HB	1:G:140:ILE:HD11	2.02	0.42
1:E:240:ASN:HD21	4:E:601:PG4:H22	1.84	0.42
1:G:497:ASN:HB2	1:H:457:ILE:HG23	2.01	0.42
1:C:431:ILE:HG23	1:C:442:TRP:CE2	2.54	0.41
1:C:276:ILE:HB	1:C:431:ILE:HG22	2.01	0.41
1:E:276:ILE:HB	1:E:431:ILE:HG22	2.02	0.41
1:D:8:GLN:HA	1:D:9:PRO:HD3	1.93	0.41
1:E:337:PRO:O	1:E:338:ASN:HB3	2.21	0.41
1:B:419:TRP:O	1:B:422:GLU:HG2	2.20	0.41
1:D:389:LEU:HB2	5:D:748:HOH:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:412:ASN:O	1:C:415:GLU:HG2	2.20	0.41
1:H:412:ASN:O	1:H:415:GLU:HG2	2.21	0.41
1:G:240:ASN:HD21	2:G:601:PGE:C5	2.34	0.41
1:B:454:ASN:HB3	1:B:457:ILE:HG13	2.01	0.41
1:A:478:ARG:C	1:A:487:GLN:HE22	2.25	0.41
1:B:140:ILE:HD11	1:C:151:ILE:HB	2.03	0.41
1:G:26:VAL:HG22	1:G:55:ALA:HB2	2.02	0.41
1:H:71:TRP:CE2	1:H:75:ALA:HB2	2.56	0.41
1:E:498:TYR:CD2	1:G:440:PHE:HB2	2.55	0.40
1:F:4:LEU:HD23	1:F:48:PRO:HB2	2.02	0.40
1:H:291:LEU:HD11	1:H:329:ILE:HD11	2.02	0.40
1:E:124:ASP:HB3	1:E:464:ILE:HG12	2.03	0.40
1:G:315:HIS:CD2	1:G:409:LYS:HG2	2.56	0.40
1:C:189:TRP:CH2	1:C:199:SER:HA	2.57	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	510/513 (99%)	496 (97%)	13 (2%)	1 (0%)	43	27
1	B	511/513 (100%)	496 (97%)	14 (3%)	1 (0%)	43	27
1	C	508/513 (99%)	492 (97%)	15 (3%)	1 (0%)	43	27
1	D	508/513 (99%)	489 (96%)	17 (3%)	2 (0%)	30	15
1	E	507/513 (99%)	492 (97%)	14 (3%)	1 (0%)	43	27
1	F	509/513 (99%)	496 (97%)	12 (2%)	1 (0%)	43	27
1	G	509/513 (99%)	493 (97%)	14 (3%)	2 (0%)	30	15
1	H	509/513 (99%)	494 (97%)	14 (3%)	1 (0%)	43	27
All	All	4071/4104 (99%)	3948 (97%)	113 (3%)	10 (0%)	43	27

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	480	SER
1	C	480	SER
1	D	480	SER
1	E	480	SER
1	F	480	SER
1	G	480	SER
1	H	480	SER
1	A	480	SER
1	D	399	GLU
1	G	399	GLU

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	395/410 (96%)	393 (100%)	2 (0%)	81	75
1	B	388/410 (95%)	385 (99%)	3 (1%)	73	64
1	C	392/410 (96%)	389 (99%)	3 (1%)	73	64
1	D	385/410 (94%)	383 (100%)	2 (0%)	81	75
1	E	392/410 (96%)	389 (99%)	3 (1%)	73	64
1	F	394/410 (96%)	391 (99%)	3 (1%)	73	64
1	G	389/410 (95%)	386 (99%)	3 (1%)	73	64
1	H	393/410 (96%)	389 (99%)	4 (1%)	68	56
All	All	3128/3280 (95%)	3105 (99%)	23 (1%)	76	67

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

Mol	Chain	Res	Type
1	A	297	THR
1	A	401	PHE
1	B	295	VAL
1	B	297	THR

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Mol	Chain	Res	Type
1	B	400	THR
1	C	297	THR
1	C	398	THR
1	C	401	PHE
1	D	297	THR
1	D	401	PHE
1	E	297	THR
1	E	401	PHE
1	E	436	LEU
1	F	47	GLU
1	F	295	VAL
1	F	297	THR
1	G	30	SER
1	G	297	THR
1	G	401	PHE
1	H	295	VAL
1	H	297	THR
1	H	358	GLU
1	H	401	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	GLN
1	A	46	ASN
1	A	153	GLN
1	A	155	ASN
1	A	213	ASN
1	B	98	GLN
1	B	155	ASN
1	B	320	ASN
1	C	98	GLN
1	C	155	ASN
1	C	412	ASN
1	D	46	ASN
1	D	153	GLN
1	D	155	ASN
1	D	259	GLN
1	E	153	GLN
1	E	155	ASN
1	F	46	ASN
1	F	155	ASN

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Mol	Chain	Res	Type
1	G	10	GLN
1	G	46	ASN
1	G	54	GLN
1	G	153	GLN
1	G	155	ASN
1	G	379	ASN
1	H	155	ASN
1	H	379	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

17 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	PGE	F	601	-	9,9,9	0.31	0	8,8,8	0.35	0
2	PGE	G	601	-	9,9,9	0.32	0	8,8,8	0.34	0
2	PGE	B	601	-	9,9,9	0.29	0	8,8,8	0.39	0
4	PG4	H	601	-	12,12,12	0.71	0	11,11,11	0.73	0
2	PGE	A	601	-	9,9,9	0.38	0	8,8,8	0.48	0
3	UN1	F	602	-	9,10,10	0.95	0	9,12,12	1.00	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	PGE	D	601	-	9,9,9	0.34	0	8,8,8	0.34	0
2	PGE	H	602	-	9,9,9	0.66	0	8,8,8	0.67	0
2	PGE	C	601	-	9,9,9	0.31	0	8,8,8	0.37	0
3	UN1	C	602	-	9,10,10	0.96	0	9,12,12	0.99	0
3	UN1	H	603	-	9,10,10	0.99	0	9,12,12	1.00	0
3	UN1	G	602	-	9,10,10	0.92	0	9,12,12	0.89	0
3	UN1	B	602	-	9,10,10	0.95	0	9,12,12	1.04	0
4	PG4	E	601	-	12,12,12	0.69	0	11,11,11	0.72	0
3	UN1	E	602	-	9,10,10	1.01	0	9,12,12	0.93	0
3	UN1	A	602	-	9,10,10	0.96	0	9,12,12	0.91	0
3	UN1	D	602	-	9,10,10	0.97	0	9,12,12	0.94	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
2	PGE	F	601	-	-	0/7/7/7	-
2	PGE	G	601	-	-	2/7/7/7	-
2	PGE	B	601	-	-	0/7/7/7	-
4	PG4	H	601	-	-	2/10/10/10	-
2	PGE	A	601	-	-	2/7/7/7	-
3	UN1	F	602	-	-	1/10/10/10	-
2	PGE	D	601	-	-	4/7/7/7	-
2	PGE	H	602	-	-	1/7/7/7	-
2	PGE	C	601	-	-	3/7/7/7	-
3	UN1	C	602	-	-	2/10/10/10	-
3	UN1	H	603	-	-	1/10/10/10	-
3	UN1	G	602	-	-	2/10/10/10	-
3	UN1	B	602	-	-	2/10/10/10	-
4	PG4	E	601	-	-	0/10/10/10	-
3	UN1	E	602	-	-	2/10/10/10	-
3	UN1	A	602	-	-	4/10/10/10	-
3	UN1	D	602	-	-	3/10/10/10	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (31) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	601	PGE	O2-C3-C4-O3
2	D	601	PGE	O2-C3-C4-O3
2	G	601	PGE	O1-C1-C2-O2
2	D	601	PGE	O1-C1-C2-O2
2	D	601	PGE	O3-C5-C6-O4
2	H	602	PGE	O3-C5-C6-O4
3	C	602	UN1	O-C-CA-N
3	E	602	UN1	O-C-CA-N
3	F	602	UN1	OXT-C-CA-N
2	D	601	PGE	C4-C3-O2-C2
2	C	601	PGE	C3-C4-O3-C5
4	H	601	PG4	C8-C7-O4-C6
2	G	601	PGE	C6-C5-O3-C4
2	C	601	PGE	C6-C5-O3-C4
2	A	601	PGE	O1-C1-C2-O2
3	A	602	UN1	O-C-CA-N
3	B	602	UN1	O-C-CA-N
3	G	602	UN1	O-C-CA-N
3	C	602	UN1	OXT-C-CA-N
3	D	602	UN1	OXT-C-CA-N
3	E	602	UN1	OXT-C-CA-N
2	A	601	PGE	C1-C2-O2-C3
4	H	601	PG4	C5-C6-O4-C7
3	B	602	UN1	OXT-C-CA-N
3	A	602	UN1	OXT-C-CA-N
3	G	602	UN1	OXT-C-CA-N
3	A	602	UN1	C6-C1-C1'-O2'
3	D	602	UN1	C6-C1-C1'-O2'
3	H	603	UN1	OXT-C-CA-N
3	A	602	UN1	C6-C1-C1'-O1'
3	D	602	UN1	C6-C1-C1'-O1'

There are no ring outliers.

5 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	601	PGE	3	0
2	A	601	PGE	4	0
2	D	601	PGE	1	0
3	H	603	UN1	1	0
4	E	601	PG4	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

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(Å²)	Q<0.9	
1	A	509/513 (99%)	-0.10	3 (0%)	85	89	10, 24, 38, 51	3 (0%)
1	B	509/513 (99%)	-0.15	5 (0%)	79	84	11, 21, 37, 54	4 (0%)
1	C	508/513 (99%)	-0.17	4 (0%)	82	86	11, 21, 35, 54	2 (0%)
1	D	509/513 (99%)	0.05	10 (1%)	65	71	12, 25, 47, 58	1 (0%)
1	E	508/513 (99%)	-0.20	3 (0%)	85	89	12, 21, 33, 44	1 (0%)
1	F	509/513 (99%)	-0.13	3 (0%)	85	89	13, 22, 37, 51	2 (0%)
1	G	509/513 (99%)	-0.17	3 (0%)	85	89	11, 23, 34, 54	2 (0%)
1	H	509/513 (99%)	-0.10	3 (0%)	85	89	9, 23, 40, 53	2 (0%)
All	All	4070/4104 (99%)	-0.12	34 (0%)	82	86	9, 22, 39, 58	17 (0%)

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	3	THR	4.0
1	B	2	SER	3.8
1	C	337	PRO	3.6
1	D	398	THR	3.5
1	G	3	THR	3.4
1	D	375	ASP	3.3
1	C	399	GLU	3.0
1	F	338	ASN	3.0
1	C	401	PHE	2.9
1	B	401	PHE	2.9
1	F	2	SER	2.8
1	H	57	VAL	2.8
1	H	3	THR	2.7
1	A	436	LEU	2.6
1	B	398	THR	2.6
1	D	360	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	401	PHE	2.5
1	E	510	PHE	2.5
1	C	398	THR	2.4
1	G	398	THR	2.3
1	D	355	GLY	2.3
1	B	402	ALA	2.2
1	D	396	ALA	2.2
1	F	401	PHE	2.2
1	A	511	GLN	2.2
1	B	57	VAL	2.2
1	D	511	GLN	2.1
1	D	327	ALA	2.1
1	D	3	THR	2.1
1	E	338	ASN	2.1
1	E	398	THR	2.1
1	D	337	PRO	2.1
1	G	399	GLU	2.1
1	H	511	GLN	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 oligosaccharides 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
2	PGE	G	601	10/10	0.86	0.13	33,39,41,42	0
2	PGE	D	601	10/10	0.87	0.13	27,36,40,41	0
2	PGE	A	601	10/10	0.88	0.12	30,34,40,42	0
2	PGE	C	601	10/10	0.89	0.12	28,34,40,42	0
4	PG4	E	601	13/13	0.89	0.11	29,35,44,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	UN1	A	602	11/11	0.90	0.10	25,35,43,46	0
3	UN1	D	602	11/11	0.90	0.11	26,28,46,50	0
3	UN1	E	602	11/11	0.90	0.09	23,31,35,36	0
3	UN1	H	603	11/11	0.90	0.09	24,30,37,45	0
2	PGE	H	602	10/10	0.90	0.12	35,40,46,51	0
3	UN1	F	602	11/11	0.92	0.09	26,28,33,38	0
3	UN1	G	602	11/11	0.92	0.08	24,29,35,39	0
2	PGE	F	601	10/10	0.92	0.09	26,29,32,33	0
3	UN1	B	602	11/11	0.92	0.08	20,25,37,39	0
2	PGE	B	601	10/10	0.93	0.10	28,32,37,38	0
3	UN1	C	602	11/11	0.93	0.08	21,23,35,36	0
4	PG4	H	601	13/13	0.93	0.09	29,32,43,45	0

6.5 Other polymers [i](#)

There are no such residues in this entry.