



Full wwPDB X-ray Structure Validation Report ⓘ

May 27, 2025 – 06:16 PM JST

PDB ID : 9J4Y / pdb_00009j4y
Title : Crystal Structure of the L322F mutant of Omega Transaminase TA_2799 from Pseudomonas putida KT2440
Authors : Das, P.; Bhaumik, P.
Deposited on : 2024-08-10
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 Phenix2.0rc1
Mogul : 1.8.5 (274361), CSD as541be (2020)
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

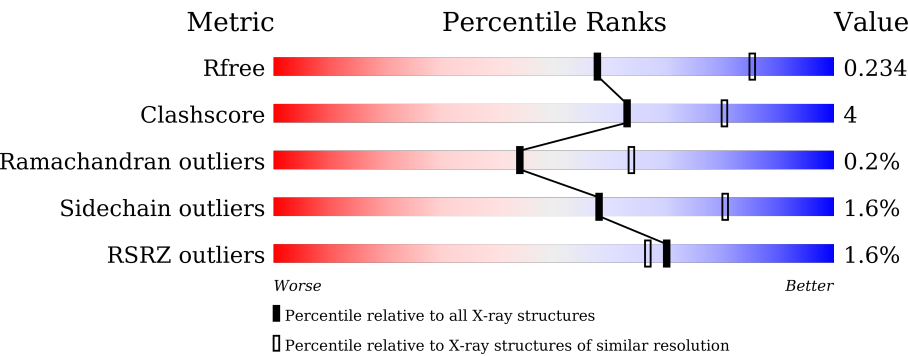
1 Overall quality at a glance i

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.



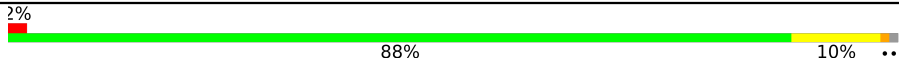
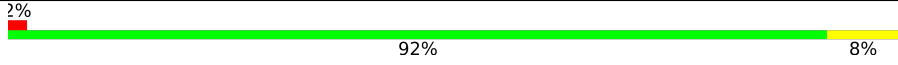
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	5504 (2.50-2.50)
Clashscore	180529	6282 (2.50-2.50)
Ramachandran outliers	177936	6191 (2.50-2.50)
Sidechain outliers	177891	6193 (2.50-2.50)
RSRZ outliers	164620	5504 (2.50-2.50)

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	459	<div><div>2%</div><div>90%</div><div>9%</div><div>..</div></div>
1	B	459	<div><div>2%</div><div>87%</div><div>11%</div><div>..</div></div>
1	C	459	<div><div>%</div><div>88%</div><div>11%</div><div>.</div></div>
1	D	459	<div><div>%</div><div>89%</div><div>9%</div><div>..</div></div>
1	E	459	<div><div>2%</div><div>90%</div><div>9%</div><div>..</div></div>
1	F	459	<div><div>%</div><div>88%</div><div>9%</div><div>..</div></div>

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Mol	Chain	Length	Quality of chain
1	G	459	 2% 88% 10% **
1	H	459	 2% 92% 8% •

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
3	EDO	B	501	-	-	X	-
3	EDO	B	502	-	-	X	-
3	EDO	B	503	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 28374 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 Aminotransferase, class III.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	456	Total	C	N	O	S	0	0	0
			3499	2233	617	638	11			
1	B	453	Total	C	N	O	S	0	2	0
			3489	2228	617	633	11			
1	C	456	Total	C	N	O	S	0	0	0
			3499	2233	617	638	11			
1	D	454	Total	C	N	O	S	0	0	0
			3483	2224	613	635	11			
1	E	455	Total	C	N	O	S	0	2	0
			3504	2236	620	637	11			
1	F	452	Total	C	N	O	S	0	1	0
			3470	2214	612	633	11			
1	G	455	Total	C	N	O	S	0	1	0
			3498	2232	619	636	11			
1	H	456	Total	C	N	O	S	0	1	0
			3505	2237	618	639	11			

There are 8 discrepancies between the modelled and reference sequences:

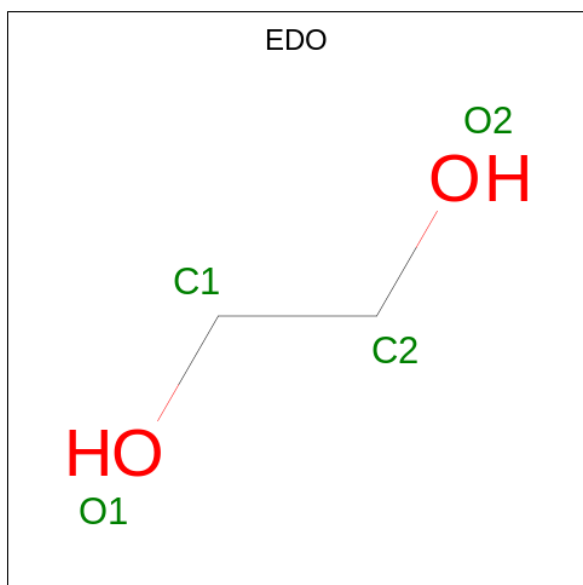
Chain	Residue	Modelled	Actual	Comment	Reference
A	322	PHE	LEU	engineered mutation	UNP Q88J50
B	322	PHE	LEU	engineered mutation	UNP Q88J50
C	322	PHE	LEU	engineered mutation	UNP Q88J50
D	322	PHE	LEU	engineered mutation	UNP Q88J50
E	322	PHE	LEU	engineered mutation	UNP Q88J50
F	322	PHE	LEU	engineered mutation	UNP Q88J50
G	322	PHE	LEU	engineered mutation	UNP Q88J50
H	322	PHE	LEU	engineered mutation	UNP Q88J50

- Molecule 2 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C₄H₁₀O₃).



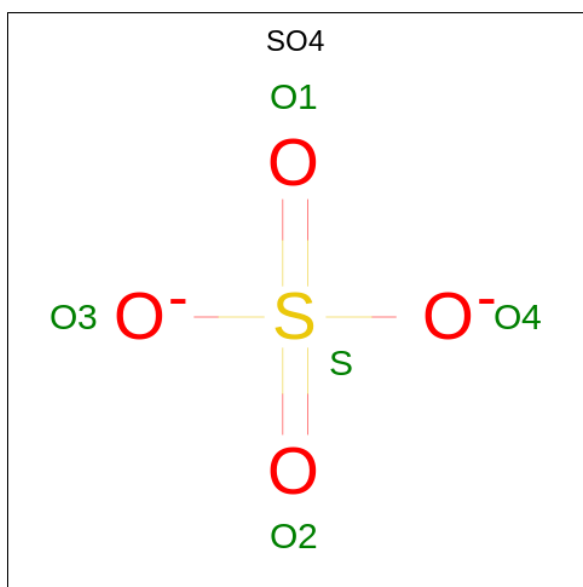
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			7	4	3		
2	C	1	Total	C	O	0	0
			7	4	3		
2	C	1	Total	C	O	0	0
			7	4	3		
2	G	1	Total	C	O	0	0
			7	4	3		

- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	C	1	Total C O 4 2 2	0	0
3	D	1	Total C O 4 2 2	0	0
3	E	1	Total C O 4 2 2	0	0
3	F	1	Total C O 4 2 2	0	0
3	H	1	Total C O 4 2 2	0	0

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



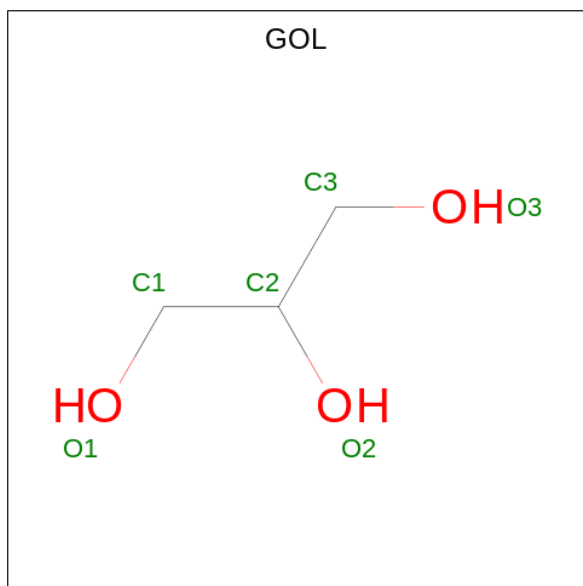
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0

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

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	C	1	Total	C	O	0	0
			6	3	3		

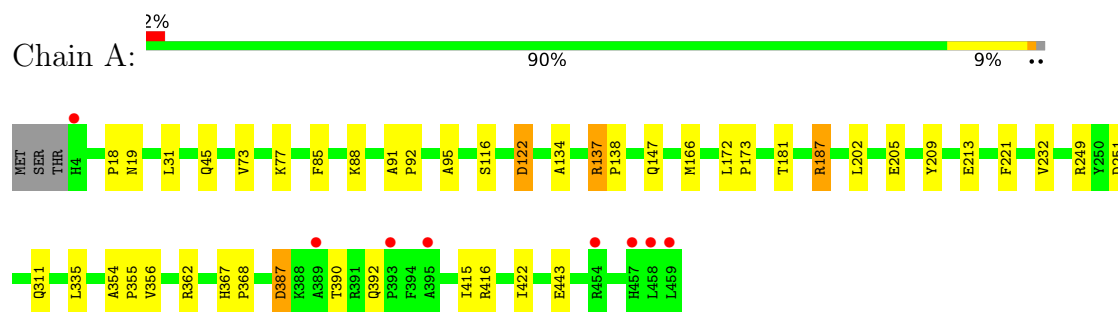
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	48	Total 48	O 48	0	0
6	B	32	Total 32	O 32	0	0
6	C	59	Total 59	O 59	0	0
6	D	55	Total 55	O 55	0	0
6	E	23	Total 23	O 23	0	0
6	F	27	Total 27	O 27	0	0
6	G	29	Total 29	O 29	0	0
6	H	25	Total 25	O 25	0	0

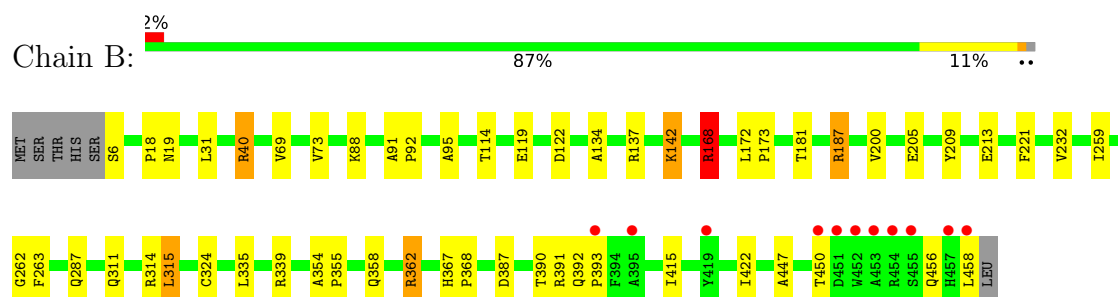
3 Residue-property plots [i](#)

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.

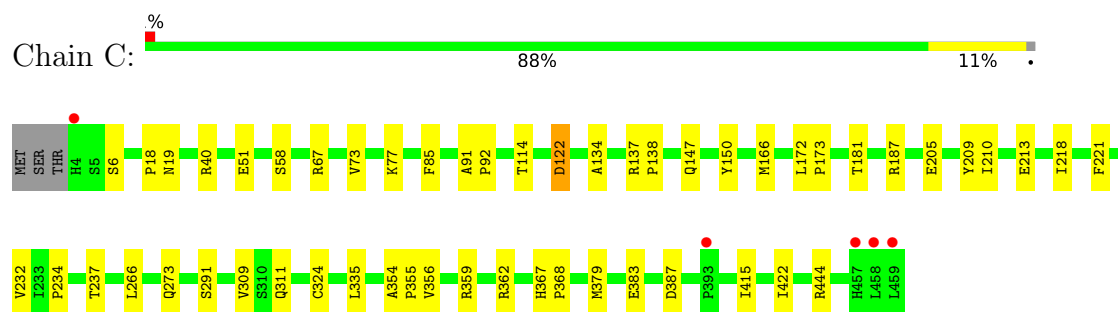
- Molecule 1: Aminotransferase, class III



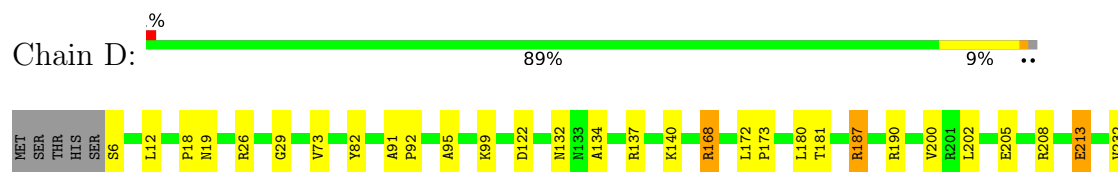
- Molecule 1: Aminotransferase, class III

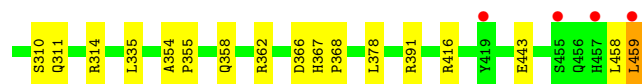


- Molecule 1: Aminotransferase, class III

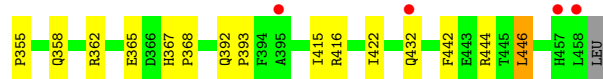
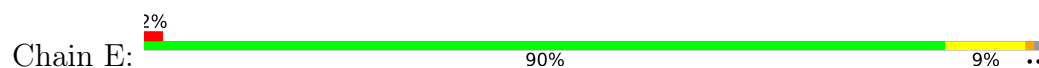


- Molecule 1: Aminotransferase, class III

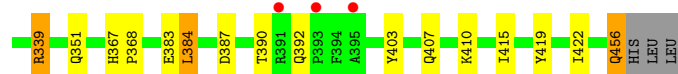
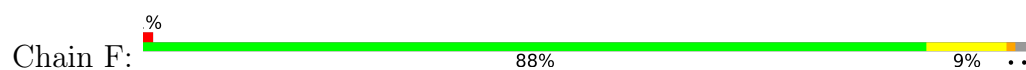




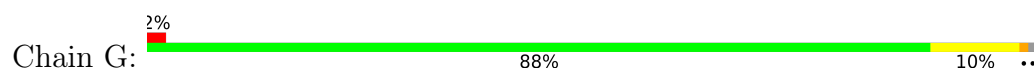
- Molecule 1: Aminotransferase, class III



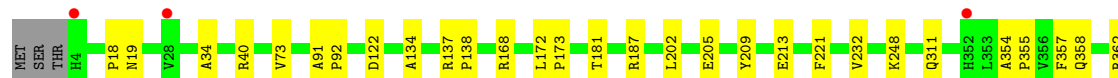
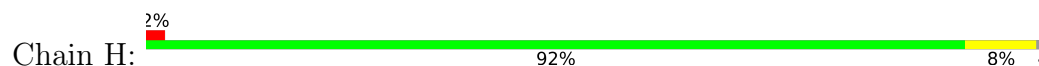
- Molecule 1: Aminotransferase, class III



- Molecule 1: Aminotransferase, class III



- Molecule 1: Aminotransferase, class III



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	119.16Å 121.44Å 147.41Å 90.00° 111.88° 90.00°	Depositor
Resolution (Å)	39.48 – 2.50 39.48 – 2.50	Depositor EDS
% Data completeness (in resolution range)	98.9 (39.48-2.50) 98.9 (39.48-2.50)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.53 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.8.0430	Depositor
R, R_{free}	0.194 , 0.233 0.200 , 0.234	Depositor DCC
R_{free} test set	6663 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	35.4	Xtriage
Anisotropy	0.064	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 28.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.000 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	28374	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 36.37 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 5.0535e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: PEG, EDO, GOL, SO4

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	0.59	0/3586	0.94	3/4884 (0.1%)
1	B	0.59	0/3582	0.95	3/4879 (0.1%)
1	C	0.59	0/3586	0.93	3/4884 (0.1%)
1	D	0.58	0/3569	0.94	1/4861 (0.0%)
1	E	0.58	0/3597	0.94	2/4899 (0.0%)
1	F	0.58	0/3558	0.96	2/4846 (0.0%)
1	G	0.56	0/3588	0.92	0/4887
1	H	0.56	0/3595	0.95	1/4897 (0.0%)
All	All	0.58	0/28661	0.94	15/39037 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	B	0	5
1	C	0	4
1	D	0	3
1	E	0	4
1	F	0	4
1	G	0	5
1	H	0	3
All	All	0	31

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	168	ARG	CA-CB-CG	6.91	127.92	114.10
1	E	4	HIS	CA-CB-CG	6.51	120.31	113.80
1	C	122	ASP	CA-CB-CG	6.05	118.65	112.60
1	B	339	ARG	CB-CG-CD	5.92	124.93	111.30
1	A	122	ASP	CA-CB-CG	5.70	118.30	112.60
1	A	443	GLU	CB-CG-CD	-5.59	103.10	112.60
1	D	366	ASP	CA-CB-CG	5.55	118.15	112.60
1	B	142	LYS	CB-CG-CD	5.47	123.87	111.30
1	F	456	GLN	CB-CA-C	5.17	119.93	110.10
1	E	365	GLU	CB-CG-CD	5.16	121.37	112.60
1	H	410	LYS	CG-CD-CE	5.15	123.14	111.30
1	A	387	ASP	CA-CB-CG	5.12	117.72	112.60
1	C	85	PHE	CA-CB-CG	5.09	118.89	113.80
1	F	419	TYR	CB-CA-C	5.06	120.50	110.42
1	C	387	ASP	CA-CB-CG	5.01	117.61	112.60

There are no chirality outliers.

All (31) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	187	ARG	Sidechain
1	A	249	ARG	Sidechain
1	A	416	ARG	Sidechain
1	B	137	ARG	Sidechain
1	B	168	ARG	Sidechain
1	B	362	ARG	Sidechain
1	B	40[A]	ARG	Sidechain
1	B	40[B]	ARG	Sidechain
1	C	137	ARG	Sidechain
1	C	359	ARG	Sidechain
1	C	40	ARG	Sidechain
1	C	444	ARG	Sidechain
1	D	168	ARG	Sidechain
1	D	208	ARG	Sidechain
1	D	416	ARG	Sidechain
1	E	137	ARG	Sidechain
1	E	168	ARG	Sidechain
1	E	416	ARG	Sidechain
1	E	444	ARG	Sidechain
1	F	137	ARG	Sidechain
1	F	339	ARG	Sidechain
1	F	40[A]	ARG	Sidechain
1	F	40[B]	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	G	168[A]	ARG	Sidechain
1	G	168[B]	ARG	Sidechain
1	G	362	ARG	Sidechain
1	G	40	ARG	Sidechain
1	G	454	ARG	Sidechain
1	H	137	ARG	Sidechain
1	H	168	ARG	Sidechain
1	H	40	ARG	Sidechain

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	3499	0	3457	29	0
1	B	3489	0	3454	47	0
1	C	3499	0	3457	30	0
1	D	3483	0	3445	32	0
1	E	3504	0	3467	23	0
1	F	3470	0	3434	31	0
1	G	3498	0	3459	29	0
1	H	3505	0	3465	19	0
2	A	7	0	10	1	0
2	C	14	0	20	2	0
2	G	7	0	10	0	0
3	A	8	0	12	2	0
3	B	12	0	18	17	0
3	C	4	0	6	3	0
3	D	4	0	6	2	0
3	E	4	0	6	1	0
3	F	4	0	6	1	0
3	H	4	0	6	1	0
4	A	5	0	0	0	0
4	B	10	0	0	0	0
4	C	5	0	0	0	0
4	D	10	0	0	0	0
4	E	5	0	0	0	0
4	F	5	0	0	0	0
4	G	10	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	H	5	0	0	0	0
5	C	6	0	8	0	0
6	A	48	0	0	1	0
6	B	32	0	0	3	0
6	C	59	0	0	2	0
6	D	55	0	0	3	0
6	E	23	0	0	0	0
6	F	27	0	0	0	0
6	G	29	0	0	0	0
6	H	25	0	0	0	0
All	All	28374	0	27746	217	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 4.

All (217) 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:G:263:PHE:HA	1:G:269:MET:HE2	1.37	1.06
1:E:257:ASP:HA	1:E:283:VAL:HG12	1.44	0.98
1:B:324:CYS:O	3:B:501:EDO:H21	1.71	0.90
1:F:403:TYR:CZ	1:F:407:GLN:HG3	2.07	0.90
1:B:200:VAL:HG13	1:F:138:PRO:HG3	1.59	0.84
1:C:237:THR:HG23	2:C:502:PEG:H42	1.60	0.83
1:C:324:CYS:O	3:C:503:EDO:H21	1.78	0.82
1:D:99:LYS:HE2	6:D:605:HOH:O	1.81	0.80
1:E:208:ARG:HB2	3:E:501:EDO:O2	1.83	0.79
1:D:180:LEU:HB3	3:D:501:EDO:H12	1.66	0.78
1:B:390:THR:HG23	1:B:392:GLN:HB3	1.66	0.77
1:E:432[A]:GLN:CD	1:E:432[A]:GLN:H	1.90	0.77
1:F:390:THR:HG23	1:F:392:GLN:HB3	1.67	0.76
1:E:257:ASP:HA	1:E:283:VAL:CG1	2.17	0.74
1:F:387:ASP:OD2	1:F:390:THR:HG22	1.89	0.73
3:B:503:EDO:H22	1:D:310:SER:O	1.90	0.71
1:G:73:VAL:HG22	1:H:73:VAL:HG22	1.74	0.69
1:B:387:ASP:OD2	1:B:390:THR:HG22	1.93	0.68
1:D:202:LEU:HD22	3:D:501:EDO:H11	1.76	0.67
1:A:387:ASP:OD2	1:A:390:THR:HG22	1.93	0.66
1:D:213:GLU:HG3	6:D:632:HOH:O	1.95	0.66
1:A:45:GLN:NE2	6:A:601:HOH:O	2.28	0.66
1:B:262:GLY:O	3:B:502:EDO:H12	1.95	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:200:VAL:HG13	1:H:138:PRO:HG3	1.78	0.65
1:G:263:PHE:HA	1:G:269:MET:CE	2.21	0.65
1:C:181:THR:HG23	1:C:205:GLU:OE1	1.98	0.63
1:F:202:LEU:HD22	3:F:501:EDO:H22	1.79	0.63
1:G:384:LEU:HD23	1:G:400:LEU:HD22	1.82	0.62
1:C:73:VAL:HG22	1:D:73:VAL:HG22	1.81	0.62
1:B:114:THR:C	3:B:501:EDO:H22	2.25	0.61
1:E:442:PHE:CZ	1:E:446:LEU:HD23	2.36	0.61
1:G:362:ARG:O	1:G:365:GLU:HG3	2.01	0.61
1:B:88:LYS:NZ	6:B:603:HOH:O	2.35	0.60
1:D:137:ARG:HH11	1:D:140:LYS:HD3	1.67	0.60
1:F:187:ARG:NH2	1:F:383:GLU:OE2	2.35	0.59
1:F:351:GLN:HE21	1:F:351:GLN:HA	1.66	0.59
1:B:209:TYR:CZ	1:B:213:GLU:HG3	2.38	0.59
1:F:403:TYR:CE2	1:F:407:GLN:HG3	2.37	0.59
1:G:181:THR:HG23	1:G:205:GLU:OE2	2.03	0.59
1:A:202:LEU:HD22	3:A:502:EDO:H22	1.86	0.58
1:A:181:THR:HG23	1:A:205:GLU:OE2	2.03	0.58
1:G:209:TYR:CZ	1:G:213:GLU:HG3	2.38	0.58
1:B:181:THR:HG23	1:B:205:GLU:OE2	2.04	0.58
1:F:403:TYR:CZ	1:F:407:GLN:CG	2.85	0.58
1:C:187:ARG:NH2	1:C:383:GLU:OE2	2.37	0.57
1:H:181:THR:HG23	1:H:205:GLU:OE2	2.04	0.57
3:B:503:EDO:H11	1:D:310:SER:OG	2.05	0.57
1:G:370:VAL:O	1:G:388:LYS:HE3	2.04	0.57
1:B:390:THR:HG23	1:B:392:GLN:CB	2.35	0.57
1:D:181:THR:HG23	1:D:205:GLU:OE2	2.04	0.57
1:E:181:THR:HG23	1:E:205:GLU:OE2	2.04	0.57
1:A:137:ARG:NH2	1:A:251:ASP:OD2	2.39	0.56
1:B:392:GLN:OE1	1:B:393:PRO:HD2	2.06	0.56
1:E:73:VAL:HG22	1:F:73:VAL:HG22	1.87	0.56
1:E:209:TYR:CZ	1:E:213:GLU:HG3	2.40	0.56
1:C:138:PRO:HG3	1:G:200:VAL:HG13	1.87	0.56
1:G:269:MET:HA	1:G:269:MET:HE3	1.88	0.55
1:H:357:PHE:HD2	1:H:435:ILE:HD12	1.71	0.55
1:G:187:ARG:NH2	1:G:391:ARG:O	2.39	0.55
1:B:324:CYS:C	3:B:501:EDO:H21	2.33	0.54
1:F:181:THR:HG23	1:F:205:GLU:OE2	2.08	0.54
1:C:67:ARG:NH1	6:C:602:HOH:O	2.40	0.53
1:A:209:TYR:CZ	1:A:213:GLU:HG3	2.43	0.53
1:D:458:LEU:O	1:D:459:LEU:OXT	2.26	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:91:ALA:HB3	1:C:92:PRO:HD3	1.92	0.52
1:D:187:ARG:NH2	1:D:391:ARG:O	2.42	0.52
1:F:387:ASP:CG	1:F:390:THR:HG22	2.34	0.52
1:G:407:GLN:OE1	1:G:410:LYS:HD2	2.09	0.52
1:H:91:ALA:HB3	1:H:92:PRO:HD3	1.92	0.51
1:B:387:ASP:CG	1:B:390:THR:HG22	2.34	0.51
1:D:99:LYS:CE	6:D:605:HOH:O	2.49	0.51
1:E:91:ALA:HB3	1:E:92:PRO:HD3	1.93	0.51
1:A:387:ASP:CG	1:A:390:THR:HG22	2.35	0.51
1:F:209:TYR:CZ	1:F:213:GLU:HG3	2.45	0.51
1:B:187:ARG:NH2	1:B:391:ARG:O	2.44	0.50
1:G:91:ALA:HB3	1:G:92:PRO:HD3	1.93	0.50
1:H:202:LEU:HB3	3:H:501:EDO:H12	1.93	0.50
1:C:114:THR:C	3:C:503:EDO:H22	2.36	0.50
1:A:73:VAL:HG22	1:B:73:VAL:HG22	1.92	0.49
1:A:91:ALA:HB3	1:A:92:PRO:HD3	1.94	0.49
1:F:403:TYR:OH	1:F:407:GLN:HG3	2.12	0.49
1:B:168:ARG:NH1	1:E:190:ARG:HE	2.10	0.49
1:B:324:CYS:O	3:B:501:EDO:C2	2.53	0.48
1:E:95:ALA:HB3	1:E:335:LEU:HD11	1.93	0.48
1:G:204:ASN:OD1	1:G:208:ARG:NH1	2.45	0.48
1:B:95:ALA:HB3	1:B:335:LEU:HD11	1.95	0.48
1:E:358:GLN:OE1	1:E:362[A]:ARG:NH1	2.46	0.48
1:F:91:ALA:HB3	1:F:92:PRO:HD3	1.95	0.48
1:C:73:VAL:HG22	1:D:73:VAL:CG2	2.43	0.48
1:C:309:VAL:HG11	1:D:26:ARG:NH1	2.28	0.48
1:A:77:LYS:HE2	1:B:69:VAL:HG11	1.95	0.48
1:A:390:THR:HG23	1:A:392:GLN:CB	2.44	0.48
1:B:263:PHE:HD2	3:B:502:EDO:C2	2.27	0.48
1:D:95:ALA:HB3	1:D:335:LEU:HD11	1.96	0.48
1:G:73:VAL:CG2	1:H:73:VAL:HG22	2.44	0.48
1:A:166:MET:HE3	6:B:612:HOH:O	2.13	0.48
1:E:354:ALA:HB3	1:E:355:PRO:HD3	1.96	0.48
1:D:190:ARG:HH21	1:G:168[A]:ARG:HH11	1.62	0.48
1:B:358:GLN:OE1	1:B:362:ARG:NH1	2.47	0.47
1:G:78:GLN:HG3	1:H:34:ALA:O	2.14	0.47
1:G:134:ALA:HB2	1:G:311:GLN:CD	2.40	0.47
1:H:358:GLN:OE1	1:H:362:ARG:NH1	2.47	0.47
1:B:263:PHE:CD2	3:B:502:EDO:C2	2.98	0.47
1:C:134:ALA:HB2	1:C:311:GLN:CD	2.40	0.47
1:E:392:GLN:CD	1:E:393:PRO:HD2	2.40	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:209:TYR:CZ	1:C:213:GLU:HG3	2.50	0.47
1:B:262:GLY:HA3	3:B:502:EDO:H21	1.97	0.47
1:A:354:ALA:HB3	1:A:355:PRO:HD3	1.97	0.46
1:C:234:PRO:O	2:C:501:PEG:H32	2.15	0.46
1:A:134:ALA:HB2	1:A:311:GLN:CD	2.40	0.46
1:A:202:LEU:HB3	3:A:502:EDO:H22	1.98	0.46
1:D:358:GLN:OE1	1:D:362:ARG:NH1	2.49	0.46
3:B:503:EDO:C1	1:D:310:SER:OG	2.64	0.46
1:G:358:GLN:OE1	1:G:362:ARG:NH1	2.49	0.46
1:H:354:ALA:HB3	1:H:355:PRO:HD3	1.97	0.46
1:G:354:ALA:HB3	1:G:355:PRO:HD3	1.98	0.46
1:E:134:ALA:HB2	1:E:311:GLN:CD	2.41	0.46
1:A:95:ALA:HB3	1:A:335:LEU:HD11	1.97	0.45
1:H:209:TYR:CZ	1:H:213:GLU:HG3	2.51	0.45
1:E:367:HIS:ND1	1:E:368:PRO:HD2	2.32	0.45
1:C:266:LEU:HD21	1:C:379:MET:HE3	1.97	0.45
1:F:95:ALA:HB3	1:F:335:LEU:HD11	1.97	0.45
1:G:281:ILE:HD11	1:G:304:MET:HE2	1.99	0.45
1:H:134:ALA:HB2	1:H:311:GLN:CD	2.42	0.45
1:F:73:VAL:O	1:F:77:LYS:HG2	2.16	0.45
1:F:134:ALA:HB2	1:F:311:GLN:CD	2.41	0.45
1:B:172:LEU:HA	1:B:173:PRO:C	2.41	0.45
1:B:287:GLN:HB2	3:B:502:EDO:O1	2.17	0.45
1:H:172:LEU:HA	1:H:173:PRO:C	2.41	0.45
1:B:314:ARG:HG3	1:B:315:LEU:HD13	1.98	0.45
1:D:18:PRO:O	1:D:19:ASN:C	2.59	0.45
1:G:442:PHE:CE2	1:G:446:LEU:HD22	2.52	0.45
1:G:447:ALA:O	1:G:450:THR:OG1	2.31	0.45
1:A:116:SER:OG	1:B:119:GLU:OE2	2.34	0.45
1:B:18:PRO:O	1:B:19:ASN:C	2.60	0.44
1:B:314:ARG:HB3	1:D:314:ARG:HB3	2.00	0.44
1:C:18:PRO:O	1:C:19:ASN:C	2.58	0.44
1:D:134:ALA:HB2	1:D:311:GLN:CD	2.43	0.44
1:B:142:LYS:HE2	6:B:622:HOH:O	2.18	0.44
1:C:172:LEU:HA	1:C:173:PRO:C	2.43	0.44
1:C:73:VAL:CG2	1:D:73:VAL:HG22	2.47	0.44
1:D:172:LEU:HA	1:D:173:PRO:C	2.41	0.44
1:C:324:CYS:C	3:C:503:EDO:H21	2.42	0.44
1:F:407:GLN:OE1	1:F:410:LYS:HD2	2.18	0.44
1:D:12:LEU:HD21	1:D:29:GLY:HA2	1.98	0.44
1:A:172:LEU:HA	1:A:173:PRO:C	2.42	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:172:LEU:HA	1:E:173:PRO:C	2.42	0.44
1:B:263:PHE:CD2	3:B:502:EDO:H21	2.53	0.43
1:C:266:LEU:HD21	1:C:379:MET:CE	2.48	0.43
1:H:18:PRO:O	1:H:19:ASN:C	2.60	0.43
1:D:367:HIS:ND1	1:D:368:PRO:HD2	2.33	0.43
1:F:73:VAL:HG13	1:F:77:LYS:HE3	2.00	0.43
1:F:281:ILE:HD11	1:F:304:MET:HE2	2.01	0.43
1:D:91:ALA:HB3	1:D:92:PRO:HD3	1.99	0.43
1:E:415:ILE:HD13	1:E:422:ILE:HG23	2.01	0.43
1:D:132:ASN:OD1	1:D:137:ARG:NH1	2.52	0.43
1:F:37:ASP:O	1:F:40[A]:ARG:NH1	2.52	0.43
1:F:172:LEU:HA	1:F:173:PRO:C	2.42	0.43
1:A:18:PRO:O	1:A:19:ASN:C	2.61	0.43
1:B:263:PHE:CD2	3:B:502:EDO:H22	2.54	0.43
1:G:172:LEU:HA	1:G:173:PRO:C	2.43	0.43
1:B:91:ALA:HB3	1:B:92:PRO:HD3	1.99	0.43
1:G:367:HIS:ND1	1:G:368:PRO:HD2	2.33	0.43
1:H:367:HIS:ND1	1:H:368:PRO:HD2	2.34	0.43
1:H:415:ILE:HD13	1:H:422:ILE:HG23	2.01	0.42
1:F:18:PRO:O	1:F:19:ASN:C	2.62	0.42
1:G:415:ILE:HD13	1:G:422:ILE:HG23	2.01	0.42
1:F:367:HIS:ND1	1:F:368:PRO:HD2	2.34	0.42
1:H:221:PHE:CD1	1:H:221:PHE:C	2.97	0.42
1:A:415:ILE:HD13	1:A:422:ILE:HG23	2.01	0.42
1:G:73:VAL:HG22	1:H:73:VAL:CG2	2.45	0.42
1:A:85:PHE:CE2	1:B:19:ASN:ND2	2.88	0.42
1:A:221:PHE:CD1	1:A:221:PHE:C	2.98	0.42
1:C:210:ILE:HA	1:C:218:ILE:CD1	2.49	0.42
1:E:446:LEU:O	1:E:446:LEU:CD1	2.67	0.42
1:F:221:PHE:CD1	1:F:221:PHE:C	2.97	0.42
1:G:18:PRO:O	1:G:19:ASN:C	2.62	0.42
1:B:354:ALA:HB3	1:B:355:PRO:HD3	2.01	0.42
1:C:221:PHE:CD1	1:C:221:PHE:C	2.98	0.42
1:F:384:LEU:HD13	1:F:384:LEU:N	2.33	0.42
1:B:221:PHE:CD1	1:B:221:PHE:C	2.98	0.42
1:C:273:GLN:HB2	6:C:608:HOH:O	2.20	0.42
1:C:354:ALA:HB3	1:C:355:PRO:HD3	2.02	0.42
1:E:187:ARG:NH2	1:E:393:PRO:HD3	2.34	0.42
1:F:415:ILE:HD13	1:F:422:ILE:HG23	2.02	0.42
1:A:88:LYS:CE	1:B:31:LEU:HD23	2.50	0.41
1:B:415:ILE:HD13	1:B:422:ILE:HG23	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:221:PHE:CD1	1:G:221:PHE:C	2.98	0.41
1:E:18:PRO:O	1:E:19:ASN:C	2.62	0.41
1:B:40[B]:ARG:HG2	1:B:40[B]:ARG:HH11	1.85	0.41
1:B:134:ALA:HB2	1:B:311:GLN:CD	2.45	0.41
1:A:138:PRO:HG3	1:E:200:VAL:HG13	2.01	0.41
1:A:147:GLN:HB2	2:A:501:PEG:H11	2.02	0.41
1:A:367:HIS:ND1	1:A:368:PRO:HD2	2.35	0.41
1:E:221:PHE:CD1	1:E:221:PHE:C	2.98	0.41
1:A:31:LEU:HD23	1:B:88:LYS:HE2	2.03	0.41
1:B:447:ALA:O	1:B:450:THR:OG1	2.33	0.41
1:B:262:GLY:C	3:B:502:EDO:H12	2.46	0.41
3:B:503:EDO:C1	1:D:310:SER:HG	2.34	0.41
1:D:354:ALA:HB3	1:D:355:PRO:HD3	2.01	0.41
1:F:58:SER:HB2	1:F:291:SER:OG	2.21	0.41
1:C:354:ALA:N	1:C:355:PRO:CD	2.84	0.41
1:B:259:ILE:O	3:B:502:EDO:H11	2.21	0.41
1:B:315:LEU:HD12	1:B:315:LEU:HA	1.80	0.41
1:B:367:HIS:ND1	1:B:368:PRO:HD2	2.36	0.41
1:B:456:GLN:O	1:B:456:GLN:HG3	2.21	0.41
1:D:378:LEU:HD12	1:D:378:LEU:HA	1.98	0.41
1:F:351:GLN:HA	1:F:351:GLN:NE2	2.32	0.41
1:A:390:THR:HG23	1:A:392:GLN:HB2	2.03	0.41
1:C:51:GLU:OE1	1:D:82:TYR:OH	2.32	0.40
1:C:367:HIS:ND1	1:C:368:PRO:HD2	2.37	0.40
1:C:150:TYR:HE1	1:C:166:MET:HE2	1.86	0.40
1:F:91:ALA:N	1:F:92:PRO:CD	2.85	0.40
1:C:58:SER:HB2	1:C:291:SER:OG	2.22	0.40
1:C:415:ILE:HD13	1:C:422:ILE:HG23	2.04	0.40
1:A:91:ALA:N	1:A:92:PRO:CD	2.85	0.40
1:H:91:ALA:N	1:H:92:PRO:CD	2.84	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	454/459 (99%)	435 (96%)	18 (4%)	1 (0%)	44	64
1	B	453/459 (99%)	435 (96%)	17 (4%)	1 (0%)	44	64
1	C	454/459 (99%)	435 (96%)	18 (4%)	1 (0%)	44	64
1	D	452/459 (98%)	434 (96%)	17 (4%)	1 (0%)	44	64
1	E	455/459 (99%)	435 (96%)	19 (4%)	1 (0%)	44	64
1	F	451/459 (98%)	432 (96%)	18 (4%)	1 (0%)	44	64
1	G	454/459 (99%)	435 (96%)	18 (4%)	1 (0%)	44	64
1	H	455/459 (99%)	438 (96%)	16 (4%)	1 (0%)	44	64
All	All	3628/3672 (99%)	3479 (96%)	141 (4%)	8 (0%)	44	64

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	232	VAL
1	C	232	VAL
1	G	232	VAL
1	B	232	VAL
1	D	232	VAL
1	E	232	VAL
1	F	232	VAL
1	H	232	VAL

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	361/364 (99%)	356 (99%)	5 (1%)	62	83
1	B	360/364 (99%)	354 (98%)	6 (2%)	56	79
1	C	361/364 (99%)	354 (98%)	7 (2%)	52	77
1	D	359/364 (99%)	352 (98%)	7 (2%)	52	77

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	362/364 (100%)	356 (98%)	6 (2%)	56	79
1	F	358/364 (98%)	351 (98%)	7 (2%)	50	75
1	G	361/364 (99%)	354 (98%)	7 (2%)	52	77
1	H	362/364 (100%)	358 (99%)	4 (1%)	70	87
All	All	2884/2912 (99%)	2835 (98%)	49 (2%)	58	79

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	122	ASP
1	A	137	ARG
1	A	187	ARG
1	A	356	VAL
1	A	362	ARG
1	B	6	SER
1	B	122	ASP
1	B	168	ARG
1	B	187	ARG
1	B	315	LEU
1	B	458	LEU
1	C	6	SER
1	C	77	LYS
1	C	122	ASP
1	C	147	GLN
1	C	335	LEU
1	C	356	VAL
1	C	362	ARG
1	D	6	SER
1	D	122	ASP
1	D	168	ARG
1	D	187	ARG
1	D	213	GLU
1	D	443	GLU
1	D	459	LEU
1	E	6	SER
1	E	122	ASP
1	E	168	ARG
1	E	187	ARG
1	E	208	ARG
1	E	446	LEU
1	F	40[A]	ARG

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Mol	Chain	Res	Type
1	F	40[B]	ARG
1	F	74	GLU
1	F	122	ASP
1	F	339	ARG
1	F	384	LEU
1	F	456	GLN
1	G	27	GLU
1	G	122	ASP
1	G	168[A]	ARG
1	G	168[B]	ARG
1	G	356	VAL
1	G	384	LEU
1	G	454	ARG
1	H	122	ASP
1	H	187	ARG
1	H	248	LYS
1	H	432	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	109	ASN
1	A	293	GLN
1	A	360	HIS
1	B	278	GLN
1	B	293	GLN
1	B	409	HIS
1	C	47	ASN
1	C	110	HIS
1	C	293	GLN
1	D	24	GLN
1	D	47	ASN
1	D	133	ASN
1	D	293	GLN
1	D	432	GLN
1	E	47	ASN
1	E	66	GLN
1	E	110	HIS
1	E	133	ASN
1	E	148	GLN
1	E	351	GLN
1	F	110	HIS

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Mol	Chain	Res	Type
1	F	351	GLN
1	F	456	GLN
1	G	47	ASN
1	G	110	HIS
1	G	293	GLN
1	H	24	GLN
1	H	47	ASN
1	H	66	GLN
1	H	109	ASN
1	H	293	GLN
1	H	313	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](#)

26 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	PEG	C	501	-	6,6,6	0.52	0	5,5,5	0.49	0
3	EDO	E	501	-	3,3,3	0.23	0	2,2,2	0.53	0
4	SO4	H	502	-	4,4,4	0.42	0	6,6,6	0.12	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	EDO	H	501	-	3,3,3	0.19	0	2,2,2	0.52	0
4	SO4	E	502	-	4,4,4	0.52	0	6,6,6	0.15	0
4	SO4	A	504	-	4,4,4	0.63	0	6,6,6	0.23	0
3	EDO	F	501	-	3,3,3	0.25	0	2,2,2	0.49	0
2	PEG	G	501	-	6,6,6	0.49	0	5,5,5	0.38	0
4	SO4	B	505	-	4,4,4	0.41	0	6,6,6	0.16	0
4	SO4	D	503	-	4,4,4	0.32	0	6,6,6	0.12	0
4	SO4	G	503	-	4,4,4	0.42	0	6,6,6	0.28	0
2	PEG	A	501	-	6,6,6	0.37	0	5,5,5	0.28	0
3	EDO	C	503	-	3,3,3	0.30	0	2,2,2	0.47	0
3	EDO	B	503	-	3,3,3	0.54	0	2,2,2	0.78	0
3	EDO	B	501	-	3,3,3	0.22	0	2,2,2	0.37	0
4	SO4	F	502	-	4,4,4	0.50	0	6,6,6	0.20	0
5	GOL	C	505	-	5,5,5	0.29	0	5,5,5	0.70	0
2	PEG	C	502	-	6,6,6	0.49	0	5,5,5	0.30	0
3	EDO	B	502	-	3,3,3	0.40	0	2,2,2	0.61	0
3	EDO	A	502	-	3,3,3	0.25	0	2,2,2	0.47	0
3	EDO	D	501	-	3,3,3	0.37	0	2,2,2	0.63	0
4	SO4	B	504	-	4,4,4	0.46	0	6,6,6	0.28	0
4	SO4	D	502	-	4,4,4	0.52	0	6,6,6	0.32	0
3	EDO	A	503	-	3,3,3	0.65	0	2,2,2	0.97	0
4	SO4	G	502	-	4,4,4	0.32	0	6,6,6	0.38	0
4	SO4	C	504	-	4,4,4	0.60	0	6,6,6	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
2	PEG	C	501	-	-	2/4/4/4	-
3	EDO	B	501	-	-	0/1/1/1	-
3	EDO	E	501	-	-	1/1/1/1	-
3	EDO	F	501	-	-	0/1/1/1	-
2	PEG	C	502	-	-	1/4/4/4	-
3	EDO	B	502	-	-	1/1/1/1	-
3	EDO	D	501	-	-	0/1/1/1	-
5	GOL	C	505	-	-	4/4/4/4	-
2	PEG	G	501	-	-	2/4/4/4	-
2	PEG	A	501	-	-	2/4/4/4	-
3	EDO	C	503	-	-	0/1/1/1	-
3	EDO	A	502	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	B	503	-	-	1/1/1/1	-
3	EDO	H	501	-	-	1/1/1/1	-
3	EDO	A	503	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	505	GOL	O1-C1-C2-O2
5	C	505	GOL	O1-C1-C2-C3
5	C	505	GOL	C1-C2-C3-O3
2	A	501	PEG	O1-C1-C2-O2
3	B	503	EDO	O1-C1-C2-O2
2	A	501	PEG	O2-C3-C4-O4
5	C	505	GOL	O2-C2-C3-O3
3	H	501	EDO	O1-C1-C2-O2
2	G	501	PEG	C4-C3-O2-C2
2	G	501	PEG	O2-C3-C4-O4
3	A	503	EDO	O1-C1-C2-O2
3	B	502	EDO	O1-C1-C2-O2
3	E	501	EDO	O1-C1-C2-O2
2	C	501	PEG	C4-C3-O2-C2
2	C	502	PEG	O2-C3-C4-O4
2	C	501	PEG	C1-C2-O2-C3

There are no ring outliers.

12 monomers are involved in 30 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	501	PEG	1	0
3	E	501	EDO	1	0
3	H	501	EDO	1	0
3	F	501	EDO	1	0
2	A	501	PEG	1	0
3	C	503	EDO	3	0
3	B	503	EDO	4	0
3	B	501	EDO	4	0
2	C	502	PEG	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	502	EDO	9	0
3	A	502	EDO	2	0
3	D	501	EDO	2	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(Å ²)	Q<0.9
1	A	456/459 (99%)	-0.34	8 (1%) 67 64	19, 33, 64, 115	0
1	B	453/459 (98%)	-0.25	11 (2%) 59 56	19, 33, 71, 125	2 (0%)
1	C	456/459 (99%)	-0.47	5 (1%) 77 74	18, 29, 59, 113	0
1	D	454/459 (98%)	-0.38	4 (0%) 81 78	18, 32, 63, 103	0
1	E	455/459 (99%)	0.05	8 (1%) 67 64	21, 42, 74, 122	2 (0%)
1	F	452/459 (98%)	-0.16	4 (0%) 81 78	20, 37, 69, 101	1 (0%)
1	G	455/459 (99%)	0.06	7 (1%) 71 68	20, 43, 76, 121	1 (0%)
1	H	456/459 (99%)	0.10	10 (2%) 62 59	24, 44, 76, 123	1 (0%)
All	All	3637/3672 (99%)	-0.17	57 (1%) 70 67	18, 36, 70, 125	7 (0%)

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	458	LEU	5.5
1	B	458	LEU	4.3
1	C	458	LEU	4.0
1	B	419	TYR	3.9
1	G	458	LEU	3.6
1	F	395	ALA	3.6
1	A	458	LEU	3.6
1	G	4	HIS	3.5
1	E	4	HIS	3.2
1	B	395	ALA	3.2
1	B	457	HIS	3.1
1	C	4	HIS	3.0
1	H	4	HIS	3.0
1	C	459	LEU	2.9
1	B	455	SER	2.9
1	D	457	HIS	2.8

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Mol	Chain	Res	Type	RSRZ
1	E	395	ALA	2.8
1	C	457	HIS	2.7
1	E	352	HIS	2.7
1	D	419	TYR	2.7
1	H	28	VAL	2.7
1	A	459	LEU	2.7
1	H	393	PRO	2.6
1	B	454	ARG	2.6
1	B	453	ALA	2.6
1	E	316	GLY	2.6
1	B	452	TRP	2.5
1	D	455	SER	2.5
1	H	394	PHE	2.5
1	A	4	HIS	2.5
1	G	394	PHE	2.5
1	H	458	LEU	2.4
1	F	5	SER	2.4
1	H	352	HIS	2.4
1	F	393	PRO	2.4
1	A	457	HIS	2.3
1	D	459	LEU	2.3
1	H	457	HIS	2.3
1	G	313	GLN	2.3
1	A	393	PRO	2.3
1	G	457	HIS	2.2
1	H	369	LEU	2.2
1	H	459	LEU	2.2
1	G	395	ALA	2.2
1	A	454	ARG	2.2
1	F	391	ARG	2.2
1	A	395	ALA	2.2
1	E	432[A]	GLN	2.1
1	A	389	ALA	2.1
1	H	391	ARG	2.1
1	C	393	PRO	2.1
1	B	451	ASP	2.1
1	G	77	LYS	2.1
1	E	457	HIS	2.1
1	E	208	ARG	2.1
1	B	450	THR	2.1
1	B	393	PRO	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(\AA^2)	Q<0.9
3	EDO	B	503	4/4	0.73	0.24	69,77,79,86	0
2	PEG	G	501	7/7	0.74	0.20	55,67,71,78	0
2	PEG	C	501	7/7	0.75	0.25	46,64,69,89	0
2	PEG	C	502	7/7	0.82	0.26	44,82,85,91	0
3	EDO	A	503	4/4	0.85	0.16	33,39,47,47	0
2	PEG	A	501	7/7	0.86	0.18	40,59,79,89	0
5	GOL	C	505	6/6	0.86	0.15	38,51,55,56	0
4	SO4	B	505	5/5	0.92	0.10	59,62,65,72	0
4	SO4	D	503	5/5	0.93	0.11	56,65,72,81	0
4	SO4	G	502	5/5	0.93	0.09	47,51,67,67	0
3	EDO	E	501	4/4	0.93	0.11	25,29,30,30	0
3	EDO	B	502	4/4	0.94	0.11	35,36,39,48	0
3	EDO	A	502	4/4	0.94	0.24	55,57,72,75	0
3	EDO	C	503	4/4	0.94	0.20	28,36,37,45	0
3	EDO	B	501	4/4	0.94	0.20	38,52,59,59	0
3	EDO	D	501	4/4	0.95	0.25	40,53,61,64	0
3	EDO	H	501	4/4	0.95	0.17	41,43,46,50	0
3	EDO	F	501	4/4	0.96	0.22	34,38,44,45	0
4	SO4	G	503	5/5	0.97	0.08	29,38,50,61	0
4	SO4	E	502	5/5	0.97	0.07	23,37,40,57	0
4	SO4	F	502	5/5	0.98	0.07	23,34,39,49	0
4	SO4	H	502	5/5	0.98	0.05	30,34,41,45	0
4	SO4	B	504	5/5	0.98	0.06	33,34,38,38	0
4	SO4	C	504	5/5	0.99	0.05	20,24,36,38	0
4	SO4	D	502	5/5	0.99	0.05	23,24,29,50	0
4	SO4	A	504	5/5	0.99	0.04	26,26,32,39	0

6.5 Other polymers [i](#)

There are no such residues in this entry.