



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 10:31 AM UTC

PDB ID : 5EXF / pdb_00005exf
Title : Thermostable aldehyde dehydrogenase from *Pyrobaculum* sp.1860 complexed with NADP+
Authors : Petrova, T.; Bezsudnova, E.Y.; Boyko, K.M.; Nikolaeva, A.Y.; Rakitina, T.V.; Popov, V.O.
Deposited on : 2015-11-23
Resolution : 2.19 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

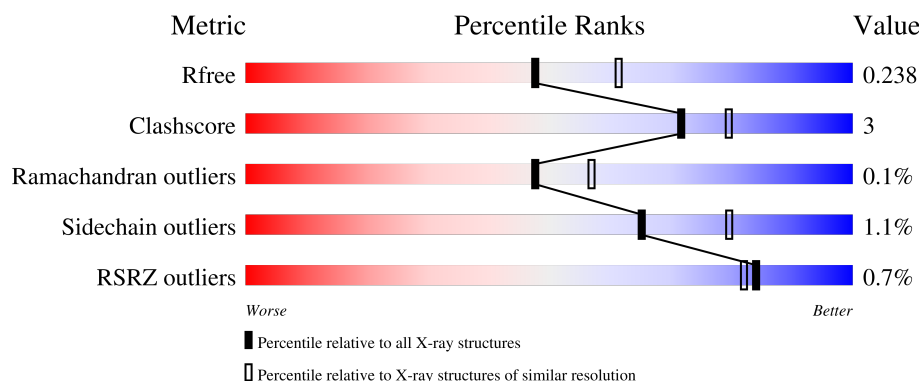
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.19 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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	491	% 93% 7%
1	B	491	% 89% 9% .
1	C	491	% 90% 10%
1	D	491	% 89% 9% .
1	E	491	% 90% 8% .

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Mol	Chain	Length	Quality of chain
1	F	491	91% 8%
1	G	491	87% 12%
1	H	491	% 90% 9%

2 Entry composition

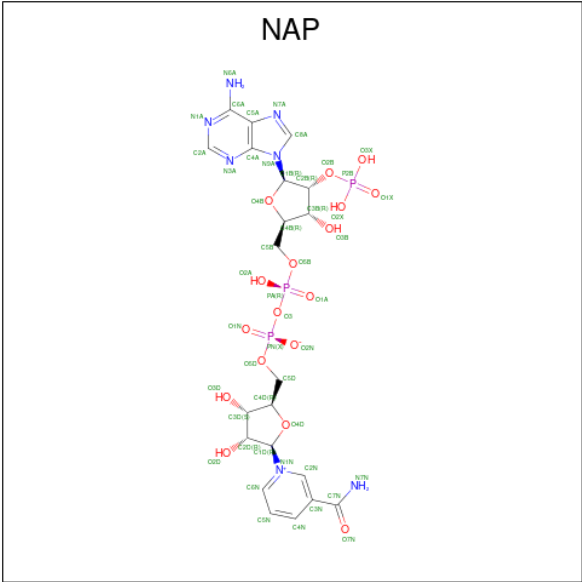
There are 4 unique types of molecules in this entry. The entry contains 33881 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Aldehyde dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	489	Total	C	N	O	S	0	5	1
			3822	2438	664	708	12			
1	B	483	Total	C	N	O	S	0	6	0
			3772	2407	654	700	11			
1	C	490	Total	C	N	O	S	0	9	1
			3838	2448	669	709	12			
1	D	483	Total	C	N	O	S	0	8	0
			3797	2422	663	701	11			
1	E	483	Total	C	N	O	S	0	5	0
			3764	2402	657	694	11			
1	F	488	Total	C	N	O	S	0	6	0
			3817	2435	664	706	12			
1	G	484	Total	C	N	O	S	0	5	0
			3784	2416	654	703	11			
1	H	487	Total	C	N	O	S	0	6	1
			3788	2418	656	702	12			

- Molecule 2 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NAP) (formula: C₂₁H₂₈N₇O₁₇P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	1
			48	21	7	17	3		
2	B	1	Total	C	N	O	P	0	1
			48	21	7	17	3		
2	C	1	Total	C	N	O	P	0	1
			48	21	7	17	3		
2	D	1	Total	C	N	O	P	0	1
			48	21	7	17	3		
2	E	1	Total	C	N	O	P	0	1
			48	21	7	17	3		
2	F	1	Total	C	N	O	P	0	1
			48	21	7	17	3		
2	G	1	Total	C	N	O	P	0	1
			48	21	7	17	3		
2	H	1	Total	C	N	O	P	0	1
			48	21	7	17	3		

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



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

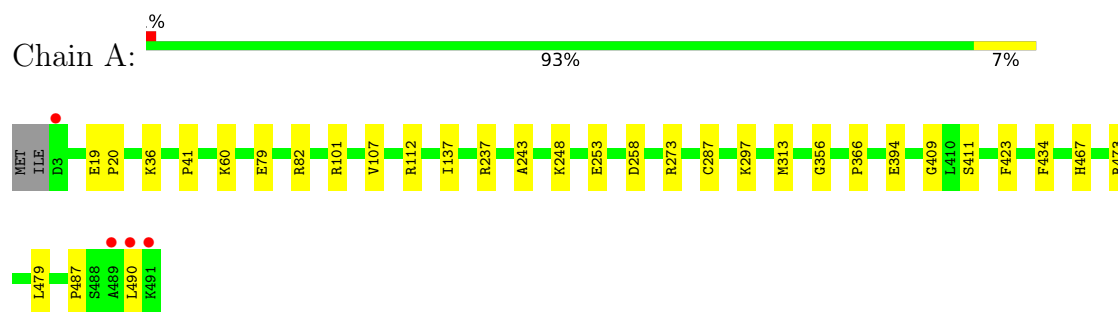
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	452	Total	O	0	0
			452	452		
4	B	391	Total	O	0	0
			391	391		
4	C	420	Total	O	0	0
			420	420		
4	D	342	Total	O	0	0
			342	342		
4	E	327	Total	O	0	0
			327	327		
4	F	393	Total	O	0	0
			393	393		
4	G	357	Total	O	0	0
			357	357		
4	H	427	Total	O	0	0
			427	427		

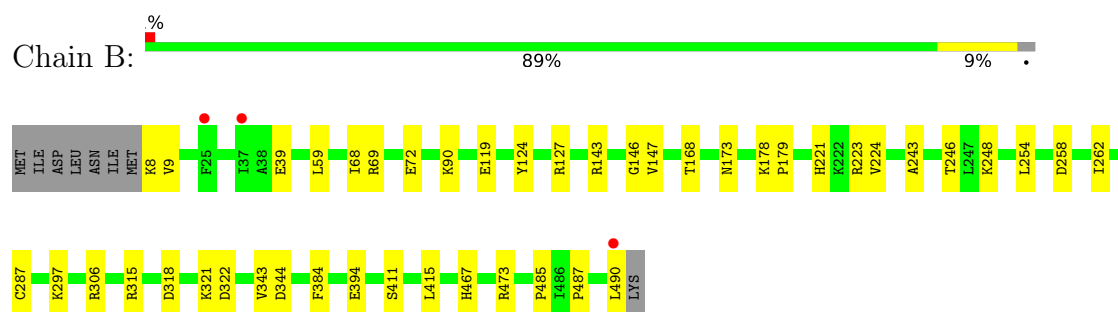
3 Residue-property plots

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.

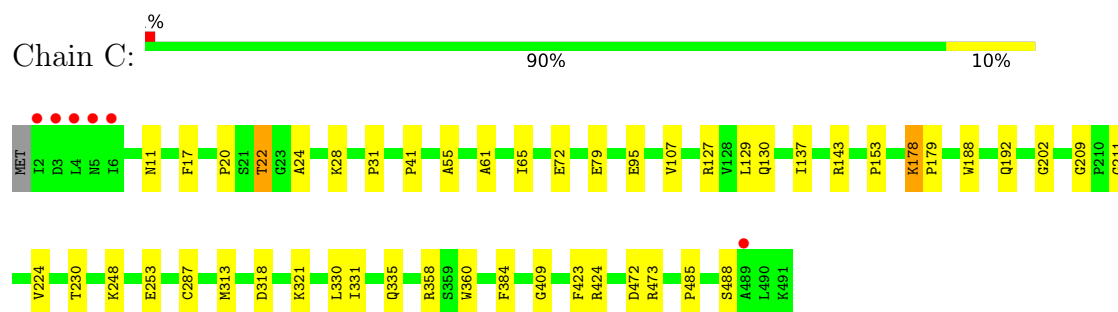
- Molecule 1: Aldehyde dehydrogenase



- Molecule 1: Aldehyde dehydrogenase

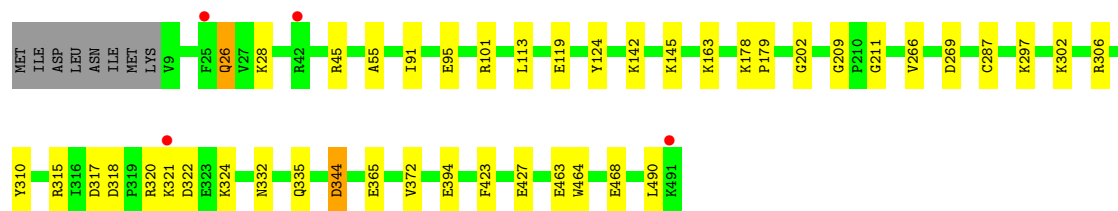


- Molecule 1: Aldehyde dehydrogenase

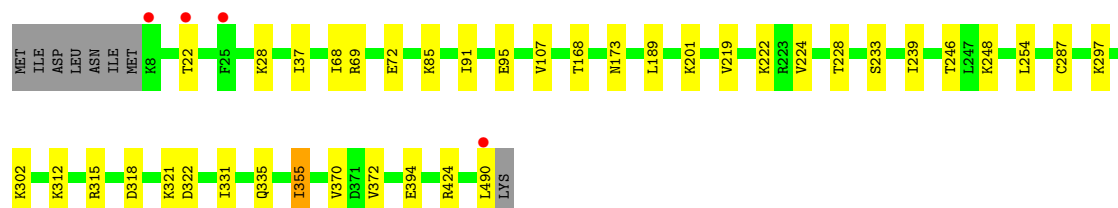
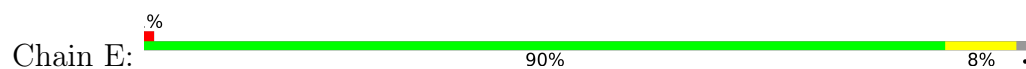


- Molecule 1: Aldehyde dehydrogenase

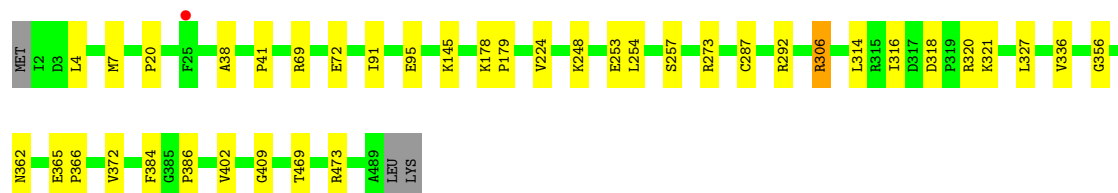
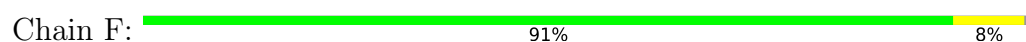




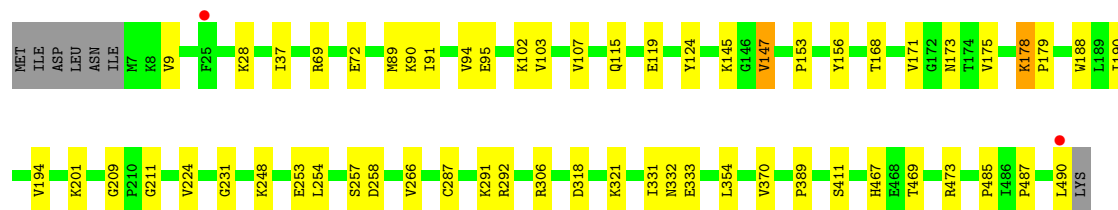
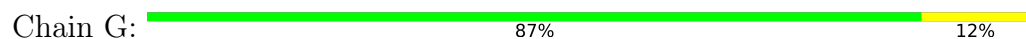
• Molecule 1: Aldehyde dehydrogenase



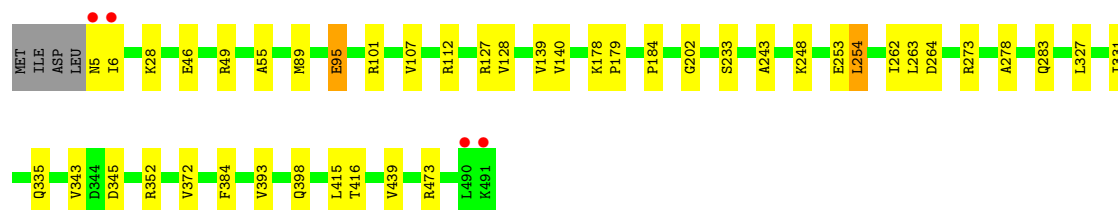
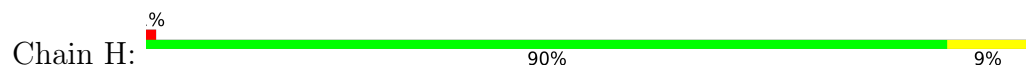
• Molecule 1: Aldehyde dehydrogenase



• Molecule 1: Aldehyde dehydrogenase



• Molecule 1: Aldehyde dehydrogenase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	185.59Å 208.72Å 164.85Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	90.97 – 2.19 90.97 – 2.19	Depositor EDS
% Data completeness (in resolution range)	97.1 (90.97-2.19) 97.2 (90.97-2.19)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.23 (at 2.18Å)	Xtrriage
Refinement program	PHENIX 1.8.4_1496	Depositor
R, R_{free}	0.206 , 0.245 0.199 , 0.238	Depositor DCC
R_{free} test set	15913 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å ²)	20.3	Xtrriage
Anisotropy	0.351	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 42.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	33881	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 46.39 % 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 1.1530e-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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NAP, GOL

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	0/3919	0.80	0/5313
1	B	0.54	0/3872	0.80	1/5253 (0.0%)
1	C	0.56	2/3944 (0.1%)	0.80	0/5349
1	D	0.52	0/3900	0.80	5/5287 (0.1%)
1	E	0.48	0/3861	0.77	0/5238
1	F	0.53	0/3917	0.76	1/5309 (0.0%)
1	G	0.47	0/3879	0.77	2/5260 (0.0%)
1	H	0.56	2/3889 (0.1%)	0.79	0/5276
All	All	0.52	4/31181 (0.0%)	0.79	9/42285 (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	B	0	2
1	D	0	2
All	All	0	4

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	129	LEU	C-N	6.83	1.42	1.33
1	C	130	GLN	C-N	-6.81	1.23	1.33
1	H	345	ASP	C-O	-6.02	1.17	1.24
1	H	343	VAL	C-O	-5.01	1.18	1.24

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	344[A]	ASP	N-CA-C	6.53	120.11	111.75
1	D	344[B]	ASP	N-CA-C	6.53	120.11	111.75
1	B	343	VAL	O-C-N	5.67	127.80	121.90
1	F	306	ARG	O-C-N	5.64	128.58	122.15
1	D	266	VAL	CB-CA-C	-5.36	105.69	111.59
1	D	209	GLY	CA-C-N	5.33	125.50	119.90
1	D	209	GLY	C-N-CA	5.33	125.50	119.90
1	G	175	VAL	N-CA-C	5.30	115.75	108.12
1	G	266	VAL	N-CA-C	5.05	115.56	110.05

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	344[A]	ASP	Mainchain
1	B	344[B]	ASP	Mainchain
1	D	344[A]	ASP	Mainchain
1	D	344[B]	ASP	Mainchain

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	3822	0	3826	24	0
1	B	3772	0	3763	33	0
1	C	3838	0	3829	32	0
1	D	3797	0	3799	29	0
1	E	3764	0	3753	23	0
1	F	3817	0	3816	25	0
1	G	3784	0	3777	32	0
1	H	3788	0	3763	25	0
2	A	48	0	13	2	0
2	B	48	0	13	3	0
2	C	48	0	13	3	0
2	D	48	0	13	2	0
2	E	48	0	13	2	0
2	F	48	0	13	4	0
2	G	48	0	13	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	H	48	0	13	3	0
3	A	6	0	8	1	0
4	A	452	0	0	3	0
4	B	391	0	0	2	0
4	C	420	0	0	5	0
4	D	342	0	0	5	0
4	E	327	0	0	3	1
4	F	393	0	0	4	0
4	G	357	0	0	0	1
4	H	427	0	0	2	0
All	All	33881	0	30438	205	1

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 3.

All (205) 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:H:233:SER:HA	1:H:254:LEU:HG	1.64	0.78
1:G:69:ARG:NH1	1:G:72[A]:GLU:OE2	2.17	0.77
1:C:358[B]:ARG:NH1	4:C:602:HOH:O	2.19	0.76
1:A:467[B]:HIS:NE2	4:A:601:HOH:O	2.20	0.75
1:A:467[B]:HIS:CE1	4:A:601:HOH:O	2.42	0.71
1:D:28[A]:LYS:HE2	1:D:95:GLU:HG3	1.73	0.69
1:D:178:LYS:NZ	1:D:179:PRO:O	2.26	0.69
1:C:72[B]:GLU:OE2	4:C:601:HOH:O	2.13	0.67
1:G:178:LYS:NZ	1:G:179:PRO:O	2.30	0.63
1:G:147:VAL:HG22	1:G:224:VAL:HA	1.80	0.62
1:G:487:PRO:HD2	1:G:490:LEU:HD12	1.81	0.62
1:B:221:HIS:HE1	1:B:223:ARG:HG3	1.65	0.61
1:B:8:LYS:NZ	1:B:39:GLU:OE2	2.35	0.60
1:C:313:MET:HE1	1:D:490:LEU:HD13	1.84	0.59
1:C:143:ARG:NH1	4:C:607:HOH:O	2.37	0.58
1:B:178:LYS:NZ	1:B:179:PRO:O	2.38	0.57
1:C:318:ASP:HB3	1:C:321:LYS:HG3	1.85	0.57
1:E:28:LYS:HE3	1:E:37:ILE:HD12	1.87	0.57
1:A:273:ARG:NH1	1:B:490:LEU:HD13	2.20	0.57
1:G:115:GLN:O	1:G:119:GLU:HG3	2.05	0.56
1:H:89:MET:HG3	1:H:107:VAL:HG21	1.87	0.56
1:H:243:ALA:HB1	1:H:248:LYS:HG3	1.88	0.56
1:A:243:ALA:HB1	1:A:248:LYS:HG3	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:423:PHE:O	1:D:427:GLU:HG2	2.07	0.55
1:G:178:LYS:HE2	1:G:209:GLY:O	2.06	0.55
1:A:237:ARG:NH2	3:A:502:GOL:O3	2.39	0.55
1:E:297:LYS:HD3	1:E:394:GLU:HG2	1.87	0.55
1:C:224:VAL:O	1:C:248:LYS:HE3	2.07	0.54
1:C:22:THR:HG23	1:C:24:ALA:H	1.71	0.54
1:A:101:ARG:HG2	1:B:485:PRO:HB2	1.90	0.54
1:D:113:LEU:HD13	1:D:163:LYS:HB2	1.91	0.53
1:H:46[A]:GLU:OE2	1:H:49:ARG:NH1	2.42	0.53
1:G:124:TYR:OH	1:G:467[A]:HIS:ND1	2.31	0.52
1:D:26:GLN:NE2	4:D:606:HOH:O	2.43	0.52
1:E:424:ARG:NH2	4:E:607:HOH:O	2.41	0.52
1:B:318:ASP:HB3	1:B:321:LYS:HG3	1.91	0.52
1:D:145:LYS:NZ	1:D:468:GLU:O	2.43	0.52
1:C:488:SER:OG	1:D:324:LYS:O	2.23	0.51
1:F:320:ARG:NH2	4:F:603:HOH:O	2.25	0.51
1:B:68:ILE:O	1:B:72[A]:GLU:HG3	2.11	0.51
1:F:318:ASP:OD1	1:F:320:ARG:HD3	2.10	0.51
1:A:479:LEU:O	1:C:424[B]:ARG:NH2	2.44	0.50
1:G:287:CYS:SG	2:G:500[A]:NAP:C4N	3.00	0.50
1:E:254:LEU:O	2:E:500[A]:NAP:H2N	2.12	0.50
1:B:143:ARG:NH1	4:B:606:HOH:O	2.44	0.50
1:B:254:LEU:O	2:B:500[A]:NAP:H2N	2.11	0.50
1:A:79[B]:GLU:OE2	1:A:82:ARG:NH1	2.45	0.50
1:B:297:LYS:HE3	1:B:394:GLU:HG2	1.94	0.49
1:E:68:ILE:O	1:E:72[A]:GLU:HG3	2.12	0.49
1:A:313:MET:HE1	1:B:490:LEU:HG	1.92	0.49
1:D:315:ARG:NH2	1:D:322:ASP:OD2	2.33	0.49
1:D:302:LYS:HE2	1:D:306:ARG:HD3	1.93	0.49
1:F:72[B]:GLU:HG3	4:F:722:HOH:O	2.12	0.49
1:F:20:PRO:HD3	1:F:41:PRO:HB3	1.95	0.49
1:C:28:LYS:HE2	1:C:95:GLU:HG3	1.94	0.49
1:E:28:LYS:HE2	1:E:95:GLU:HG3	1.95	0.48
1:F:316:ILE:HD12	1:F:365:GLU:HG2	1.94	0.48
1:E:224:VAL:O	1:E:248:LYS:HE3	2.13	0.48
1:E:219:VAL:HG21	1:E:239:ILE:HG12	1.94	0.48
1:F:145:LYS:HG3	1:F:469:THR:C	2.39	0.48
1:A:19:GLU:HB2	1:A:20:PRO:HD2	1.96	0.48
1:A:258:ASP:OD2	1:A:411:SER:HB3	2.14	0.48
1:F:224:VAL:O	1:F:248:LYS:HE3	2.14	0.48
1:G:257:SER:O	1:G:292:ARG:NH1	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:297:LYS:HD3	1:A:394:GLU:HG2	1.96	0.47
1:B:243:ALA:HB1	1:B:248:LYS:HG3	1.96	0.47
1:G:318:ASP:HB3	1:G:321:LYS:HG3	1.96	0.47
1:C:31:PRO:HB3	1:C:331:ILE:O	2.13	0.47
1:F:91:ILE:O	1:F:95:GLU:HB3	2.13	0.47
1:C:178:LYS:HE3	1:C:211:GLY:HA2	1.96	0.47
1:D:463[B]:GLU:HG2	4:D:667:HOH:O	2.14	0.47
1:G:253:GLU:HB3	2:G:500[A]:NAP:C7N	2.43	0.47
1:B:221:HIS:CE1	1:B:223:ARG:HG3	2.47	0.47
1:F:292:ARG:NH2	1:F:402:VAL:O	2.47	0.47
1:G:178:LYS:HE3	1:G:211:GLY:HA2	1.97	0.47
1:B:69:ARG:HH11	1:B:72[A]:GLU:HB2	1.80	0.47
1:G:190:ILE:O	1:G:194:VAL:HG23	2.15	0.47
1:B:262:ILE:HG12	1:B:415:LEU:HD12	1.97	0.47
1:A:287[A]:CYS:SG	2:A:501[A]:NAP:C4N	3.03	0.47
1:B:287[A]:CYS:SG	2:B:500[A]:NAP:C4N	3.03	0.46
1:C:472:ASP:OD2	1:D:464:TRP:NE1	2.44	0.46
1:E:318:ASP:HB3	1:E:321:LYS:HG3	1.97	0.46
1:B:258:ASP:OD2	1:B:411:SER:HB3	2.16	0.46
1:E:91:ILE:O	1:E:95:GLU:HB3	2.16	0.46
1:C:55:ALA:HA	1:C:202:GLY:O	2.15	0.46
1:C:178:LYS:HE2	1:C:209:GLY:O	2.16	0.45
1:A:20:PRO:HD3	1:A:41:PRO:HB3	1.98	0.45
1:C:253:GLU:HB3	2:C:500[A]:NAP:C7N	2.47	0.45
1:C:358[B]:ARG:HE	1:C:360:TRP:HZ2	1.63	0.45
1:G:258:ASP:OD2	1:G:411:SER:HB3	2.16	0.45
1:G:490:LEU:HD13	1:H:273:ARG:NH1	2.32	0.45
1:B:487:PRO:HD2	1:B:490:LEU:HD12	1.97	0.45
1:D:45:ARG:HG3	4:D:837:HOH:O	2.17	0.45
1:H:384:PHE:CE1	2:H:500[A]:NAP:H2D	2.51	0.45
1:B:224:VAL:O	1:B:248:LYS:HE3	2.17	0.45
1:C:127:ARG:NE	4:C:612:HOH:O	2.42	0.45
1:H:393:VAL:HB	1:H:398:GLN:HB3	1.98	0.45
1:B:119:GLU:HA	1:D:119:GLU:HG2	1.98	0.45
1:B:168:THR:HG22	1:B:173:ASN:HB2	1.99	0.45
1:E:85:LYS:NZ	4:E:606:HOH:O	2.37	0.45
1:H:283:GLN:HG3	1:H:327:LEU:HB3	1.99	0.45
1:C:178:LYS:NZ	1:C:179:PRO:O	2.50	0.44
1:H:352:ARG:HD2	4:H:603:HOH:O	2.17	0.44
1:F:253:GLU:HB3	2:F:500[A]:NAP:C7N	2.46	0.44
1:B:90:LYS:NZ	4:B:601:HOH:O	2.29	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:287[A]:CYS:SG	2:D:500[A]:NAP:C4N	3.05	0.44
1:D:297:LYS:HD3	1:D:394:GLU:HG2	1.99	0.44
1:B:246:THR:OG1	1:B:248:LYS:NZ	2.46	0.44
1:D:318:ASP:OD2	1:D:320:ARG:NH2	2.28	0.44
1:H:254:LEU:O	2:H:500[A]:NAP:H2N	2.18	0.44
1:D:321:LYS:HB3	1:D:321:LYS:HE3	1.89	0.44
1:E:331:ILE:HG22	1:E:335:GLN:HG3	1.99	0.44
1:B:69:ARG:HH11	1:B:72[B]:GLU:HB3	1.82	0.44
1:C:384:PHE:CE1	2:C:500[A]:NAP:H2D	2.53	0.44
1:E:287[A]:CYS:SG	2:E:500[A]:NAP:C4N	3.06	0.44
1:G:354:LEU:HD11	1:G:370:VAL:HG13	1.99	0.44
1:A:487:PRO:HD2	1:A:490:LEU:HD12	2.00	0.43
1:D:178:LYS:HE3	1:D:211:GLY:HA2	1.98	0.43
1:H:178:LYS:NZ	1:H:179:PRO:O	2.40	0.43
1:B:315:ARG:NH2	1:B:322:ASP:OD1	2.49	0.43
1:C:61:ALA:O	1:C:65:ILE:HG23	2.18	0.43
1:F:366:PRO:HA	1:F:386:PRO:O	2.19	0.43
1:F:384:PHE:CE1	2:F:500[A]:NAP:H2D	2.52	0.43
1:G:91:ILE:O	1:G:95:GLU:HB3	2.18	0.43
1:D:287[A]:CYS:HB3	2:D:500[A]:NAP:C3N	2.48	0.43
1:F:318:ASP:HB3	1:F:321:LYS:HG3	1.99	0.43
1:A:253:GLU:HB3	2:A:501[A]:NAP:N7N	2.34	0.43
1:C:20:PRO:HD3	1:C:41:PRO:HB3	2.00	0.43
1:C:79[B]:GLU:HG2	4:C:603:HOH:O	2.18	0.43
1:F:314:LEU:HD13	1:F:327:LEU:HD11	2.01	0.43
1:H:5:ASN:OD1	1:H:6:ILE:HG12	2.19	0.43
1:A:356:GLY:HA3	1:A:366:PRO:O	2.18	0.43
1:B:59:LEU:HD21	1:B:146:GLY:HA2	2.01	0.43
1:D:427:GLU:HG3	4:D:656:HOH:O	2.18	0.43
1:G:485:PRO:HB2	1:H:101:ARG:HG2	1.99	0.43
1:A:137:ILE:HD12	1:C:423:PHE:CE2	2.54	0.43
1:G:224:VAL:O	1:G:248:LYS:HE3	2.19	0.43
1:H:331:ILE:HG22	1:H:335:GLN:HG3	2.00	0.43
1:E:69[A]:ARG:HH21	1:E:72[A]:GLU:HB2	1.84	0.43
1:F:7:MET:HE3	1:F:38:ALA:HB2	2.01	0.43
1:H:127:ARG:O	1:H:140:VAL:N	2.46	0.43
1:B:124:TYR:OH	1:B:467[A]:HIS:ND1	2.36	0.42
1:F:72[A]:GLU:HG2	4:F:800:HOH:O	2.18	0.42
1:F:306:ARG:HA	1:F:306:ARG:HD2	1.72	0.42
1:G:102:LYS:HE2	1:G:156:TYR:CZ	2.54	0.42
1:E:189:LEU:HD23	1:E:189:LEU:HA	1.87	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:257:SER:OG	1:F:292:ARG:HD2	2.19	0.42
1:H:128:VAL:HG22	1:H:139:VAL:HG12	2.01	0.42
1:F:336:VAL:HG21	1:F:362:ASN:HA	2.00	0.42
1:D:365:GLU:HG2	4:D:612:HOH:O	2.19	0.42
1:A:273:ARG:HH12	1:B:490:LEU:HD22	1.85	0.42
1:B:384:PHE:CE1	2:B:500[A]:NAP:H2D	2.55	0.42
1:E:315:ARG:HH22	1:E:322:ASP:CG	2.27	0.42
1:G:89:MET:HE3	1:G:103:VAL:HG23	2.01	0.42
1:H:253:GLU:HB3	2:H:500[A]:NAP:C7N	2.50	0.42
1:C:11:ASN:O	1:C:17:PHE:HA	2.20	0.42
1:D:55:ALA:HA	1:D:202:GLY:O	2.20	0.42
1:F:287[A]:CYS:SG	2:F:500[A]:NAP:C4N	3.08	0.42
1:G:28:LYS:HE2	1:G:95:GLU:HG3	2.00	0.42
1:A:467[B]:HIS:NE2	1:B:467[B]:HIS:NE2	2.67	0.42
1:C:188:TRP:CZ2	1:C:192:GLN:NE2	2.88	0.42
1:E:168:THR:HG22	1:E:173:ASN:HB2	2.01	0.42
1:E:233:SER:HA	1:E:254:LEU:HD13	2.00	0.42
1:G:9:VAL:HB	1:G:188:TRP:CD1	2.54	0.42
1:D:269:ASP:OD1	1:D:310:TYR:OH	2.29	0.42
1:G:331:ILE:HG23	1:G:332:ASN:ND2	2.33	0.42
1:G:90:LYS:O	1:G:94:VAL:HG12	2.20	0.42
1:G:145:LYS:HG3	1:G:469:THR:C	2.45	0.42
1:G:291:LYS:O	1:G:389:PRO:HD2	2.21	0.41
1:C:153:PRO:HG3	1:C:230:THR:HG22	2.02	0.41
1:C:485:PRO:HB2	1:D:101:ARG:HG2	2.01	0.41
1:B:315:ARG:HH22	1:B:322:ASP:CG	2.28	0.41
1:D:91:ILE:O	1:D:95:GLU:HB3	2.21	0.41
1:G:91:ILE:HD13	1:G:91:ILE:HA	1.93	0.41
1:G:168:THR:HG22	1:G:173:ASN:HB2	2.02	0.41
1:H:262:ILE:HG12	1:H:415:LEU:HD12	2.02	0.41
1:H:95:GLU:OE2	1:H:184:PRO:HD2	2.20	0.41
1:D:317:ASP:OD2	1:D:321:LYS:HE2	2.20	0.41
1:G:9:VAL:HB	1:G:188:TRP:CG	2.56	0.41
1:H:28[B]:LYS:HA	1:H:28[B]:LYS:HD3	1.79	0.41
1:F:365:GLU:OE1	4:F:601:HOH:O	2.22	0.41
1:G:231:GLY:O	1:G:254:LEU:HA	2.21	0.41
1:D:332:ASN:OD1	1:D:335:GLN:HG2	2.21	0.41
1:E:85:LYS:HG2	1:E:107:VAL:CG1	2.50	0.41
1:E:222:LYS:HA	1:E:246:THR:HG21	2.03	0.41
1:E:490:LEU:HD13	1:F:273:ARG:NH1	2.36	0.41
1:F:356:GLY:HA3	1:F:366:PRO:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:28:LYS:HE3	1:G:37:ILE:HD12	2.02	0.41
1:H:263:LEU:HD12	1:H:416:THR:HB	2.03	0.41
1:C:287[A]:CYS:SG	2:C:500[A]:NAP:C4N	3.09	0.41
1:A:434:PHE:HB2	1:B:473:ARG:NH2	2.35	0.40
1:H:55:ALA:HA	1:H:202:GLY:O	2.20	0.40
1:H:112:ARG:HB3	4:H:664:HOH:O	2.21	0.40
1:A:423:PHE:CD2	1:C:137:ILE:HD12	2.56	0.40
1:D:124:TYR:CZ	1:D:142:LYS:HE3	2.56	0.40
1:F:178:LYS:NZ	1:F:179:PRO:O	2.54	0.40
1:F:254:LEU:O	2:F:500[A]:NAP:H2N	2.22	0.40
1:H:278:ALA:HB2	1:H:439:VAL:HG12	2.02	0.40
1:A:112:ARG:HB3	4:A:654:HOH:O	2.21	0.40
1:C:331:ILE:HG22	1:C:335:GLN:HG3	2.03	0.40
1:E:201:LYS:NZ	4:E:614:HOH:O	2.48	0.40
1:A:137:ILE:HD12	1:C:423:PHE:CD2	2.56	0.40
1:B:127:ARG:HA	1:B:127:ARG:HD3	1.98	0.40
1:H:264:ASP:OD1	1:H:264:ASP:N	2.51	0.40
1:E:312:LYS:HG2	1:E:355:ILE:HD11	2.03	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:871:HOH:O	4:G:912:HOH:O[4_455]	2.15	0.05

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	492/491 (100%)	474 (96%)	17 (4%)	1 (0%)	43 51
1	B	487/491 (99%)	473 (97%)	14 (3%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	497/491 (101%)	481 (97%)	15 (3%)	1 (0%)	43	51
1	D	489/491 (100%)	472 (96%)	17 (4%)	0	100	100
1	E	486/491 (99%)	470 (97%)	16 (3%)	0	100	100
1	F	492/491 (100%)	476 (97%)	15 (3%)	1 (0%)	43	51
1	G	487/491 (99%)	470 (96%)	16 (3%)	1 (0%)	43	51
1	H	491/491 (100%)	474 (96%)	17 (4%)	0	100	100
All	All	3921/3928 (100%)	3790 (97%)	127 (3%)	4 (0%)	48	57

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	409	GLY
1	C	409	GLY
1	G	153	PRO
1	F	409	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	406/408 (100%)	402 (99%)	4 (1%)	68	81
1	B	399/408 (98%)	396 (99%)	3 (1%)	73	85
1	C	405/408 (99%)	400 (99%)	5 (1%)	63	78
1	D	402/408 (98%)	400 (100%)	2 (0%)	81	90
1	E	396/408 (97%)	390 (98%)	6 (2%)	57	73
1	F	403/408 (99%)	398 (99%)	5 (1%)	63	78
1	G	400/408 (98%)	391 (98%)	9 (2%)	44	59
1	H	398/408 (98%)	394 (99%)	4 (1%)	68	81
All	All	3209/3264 (98%)	3171 (99%)	38 (1%)	65	78

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	LYS
1	A	60	LYS
1	A	107	VAL
1	A	473	ARG
1	B	9	VAL
1	B	147	VAL
1	B	306	ARG
1	C	22	THR
1	C	107	VAL
1	C	178	LYS
1	C	330	LEU
1	C	473	ARG
1	D	26	GLN
1	D	372	VAL
1	E	22	THR
1	E	228	THR
1	E	302	LYS
1	E	355	ILE
1	E	370	VAL
1	E	372	VAL
1	F	4	LEU
1	F	69[A]	ARG
1	F	69[B]	ARG
1	F	372	VAL
1	F	473	ARG
1	G	107	VAL
1	G	147	VAL
1	G	171	VAL
1	G	178	LYS
1	G	201	LYS
1	G	306	ARG
1	G	333[A]	GLU
1	G	333[B]	GLU
1	G	473	ARG
1	H	95	GLU
1	H	254	LEU
1	H	372	VAL
1	H	473	ARG

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

Mol	Chain	Res	Type
1	A	285	GLN

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Mol	Chain	Res	Type
1	D	26	GLN
1	D	192	GLN
1	E	285	GLN
1	E	362	ASN
1	F	285	GLN
1	F	417	ASN
1	G	64	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

9 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	$\# Z > 2$
3	GOL	A	502	-	5,5,5	0.34	0	5,5,5	0.52	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
3	GOL	A	502	-	-	0/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	502	GOL	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(Å ²)	Q<0.9
1	A	489/491 (99%)	-0.54	4 (0%) 82 80	8, 16, 32, 58	6 (1%)
1	B	483/491 (98%)	-0.42	3 (0%) 85 83	8, 18, 36, 50	7 (1%)
1	C	490/491 (99%)	-0.40	6 (1%) 76 74	9, 17, 33, 51	10 (2%)
1	D	483/491 (98%)	-0.20	4 (0%) 82 80	9, 21, 41, 61	9 (1%)
1	E	483/491 (98%)	-0.24	4 (0%) 82 80	10, 24, 42, 55	5 (1%)
1	F	488/491 (99%)	-0.40	1 (0%) 91 90	9, 20, 35, 55	7 (1%)
1	G	484/491 (98%)	-0.29	2 (0%) 88 87	9, 23, 37, 46	6 (1%)
1	H	487/491 (99%)	-0.41	4 (0%) 82 80	9, 19, 34, 57	7 (1%)
All	All	3887/3928 (98%)	-0.36	28 (0%) 84 82	8, 20, 37, 61	57 (1%)

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	491	LYS	6.1
1	H	491	LYS	5.4
1	H	5	ASN	4.7
1	B	490	LEU	4.4
1	G	25	PHE	4.1
1	C	2	ILE	4.1
1	E	490	LEU	3.8
1	D	491	LYS	3.8
1	D	25	PHE	3.6
1	B	25	PHE	3.6
1	H	6	ILE	3.4
1	C	6	ILE	3.3
1	C	4	LEU	3.1
1	E	25	PHE	2.7
1	C	5	ASN	2.7
1	A	490	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	H	490	LEU	2.4
1	A	3	ASP	2.4
1	C	3	ASP	2.4
1	E	22	THR	2.4
1	G	490	LEU	2.2
1	F	25	PHE	2.2
1	A	489	ALA	2.2
1	D	42	ARG	2.1
1	D	321	LYS	2.0
1	E	8	LYS	2.0
1	B	37	ILE	2.0
1	C	489	ALA	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

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
3	GOL	A	502	6/6	0.93	0.10	34,36,38,40	0
2	NAP	F	500[A]	48/48	0.96	0.08	11,21,27,32	18
2	NAP	G	500[A]	48/48	0.96	0.07	12,23,28,32	17
2	NAP	D	500[A]	48/48	0.96	0.08	10,22,30,33	17
2	NAP	E	500[A]	48/48	0.97	0.06	13,25,30,35	17
2	NAP	B	500[A]	48/48	0.97	0.06	11,18,23,26	17
2	NAP	C	500[A]	48/48	0.97	0.07	11,20,24,27	17
2	NAP	H	500[A]	48/48	0.97	0.07	11,19,27,30	18
2	NAP	A	501[A]	48/48	0.97	0.07	11,17,22,28	17

6.5 Other polymers [i](#)

There are no such residues in this entry.