



Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 01:26 AM GMT

PDB ID : 3I2B
Title : The crystal structure of human 6 Pyruvoyl Tetrahydrobiopterin Synthase
Authors : Ugochukwu, E.; Cocking, R.; Pilka, E.; Yue, W.W.; Bray, J.E.; Chaikuad, A.; Krojer, T.; Muniz, J.; von Delft, F.; Bountra, C.; Arrowsmith, C.H.; Weigelt, J.; Edwards, A.; Oppermann, U.; Structural Genomics Consortium (SGC)
Deposited on : 2009-06-29
Resolution : 2.30 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

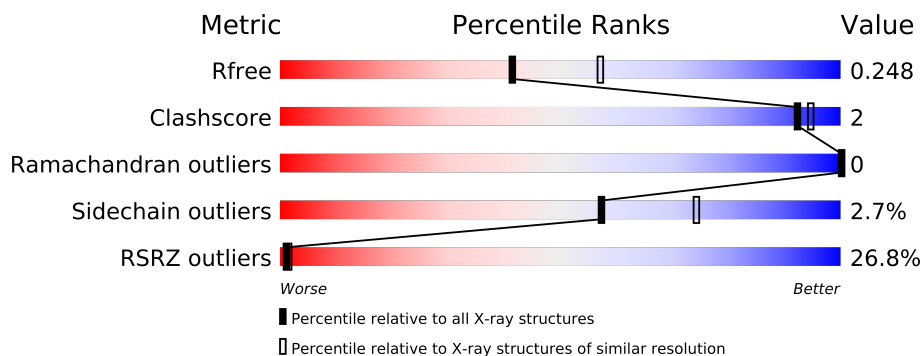
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.30 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}	66092	2929 (2.30-2.30)
Clashscore	79885	3679 (2.30-2.30)
Ramachandran outliers	78287	3642 (2.30-2.30)
Sidechain outliers	78261	3641 (2.30-2.30)
RSRZ outliers	66119	2930 (2.30-2.30)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	141	
1	B	141	
1	C	141	
1	D	141	
1	E	141	
1	F	141	
1	G	141	
1	H	141	
1	I	141	
1	J	141	
1	K	141	
1	L	141	

The following table lists non-polymeric compounds that are outliers for geometric or electron-

density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
4	MG	A	2	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 13128 atoms, of which 0 are hydrogen and 0 are deuterium.

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 6-pyruvoyl tetrahydrobiopterin synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	138	Total	C	N	O	S	0	0	0
			1080	684	185	204	7			
1	D	138	Total	C	N	O	S	0	2	0
			1099	698	184	210	7			
1	E	138	Total	C	N	O	S	0	0	0
			1064	673	178	206	7			
1	B	138	Total	C	N	O	S	0	1	0
			1093	698	186	202	7			
1	C	137	Total	C	N	O	S	0	1	0
			1071	683	179	202	7			
1	F	138	Total	C	N	O	S	0	0	0
			1071	680	182	202	7			
1	G	136	Total	C	N	O	S	0	0	0
			1040	660	179	194	7			
1	H	137	Total	C	N	O	S	0	0	0
			1045	664	176	198	7			
1	I	138	Total	C	N	O	S	0	0	0
			1084	688	185	204	7			
1	J	137	Total	C	N	O	S	0	0	0
			1063	675	180	201	7			
1	K	138	Total	C	N	O	S	0	0	0
			1051	668	179	197	7			
1	L	138	Total	C	N	O	S	0	0	0
			1079	684	182	206	7			

There are 24 discrepancies between the modelled and reference sequences:

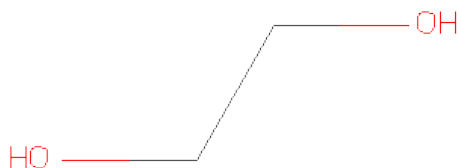
Chain	Residue	Modelled	Actual	Comment	Reference
A	5	SER	-	EXPRESSION TAG	UNP Q03393
A	6	MET	-	EXPRESSION TAG	UNP Q03393
D	5	SER	-	EXPRESSION TAG	UNP Q03393
D	6	MET	-	EXPRESSION TAG	UNP Q03393
E	5	SER	-	EXPRESSION TAG	UNP Q03393

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Chain	Residue	Modelled	Actual	Comment	Reference
E	6	MET	-	EXPRESSION TAG	UNP Q03393
B	5	SER	-	EXPRESSION TAG	UNP Q03393
B	6	MET	-	EXPRESSION TAG	UNP Q03393
C	5	SER	-	EXPRESSION TAG	UNP Q03393
C	6	MET	-	EXPRESSION TAG	UNP Q03393
F	5	SER	-	EXPRESSION TAG	UNP Q03393
F	6	MET	-	EXPRESSION TAG	UNP Q03393
G	5	SER	-	EXPRESSION TAG	UNP Q03393
G	6	MET	-	EXPRESSION TAG	UNP Q03393
H	5	SER	-	EXPRESSION TAG	UNP Q03393
H	6	MET	-	EXPRESSION TAG	UNP Q03393
I	5	SER	-	EXPRESSION TAG	UNP Q03393
I	6	MET	-	EXPRESSION TAG	UNP Q03393
J	5	SER	-	EXPRESSION TAG	UNP Q03393
J	6	MET	-	EXPRESSION TAG	UNP Q03393
K	5	SER	-	EXPRESSION TAG	UNP Q03393
K	6	MET	-	EXPRESSION TAG	UNP Q03393
L	5	SER	-	EXPRESSION TAG	UNP Q03393
L	6	MET	-	EXPRESSION TAG	UNP Q03393

- Molecule 2 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



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

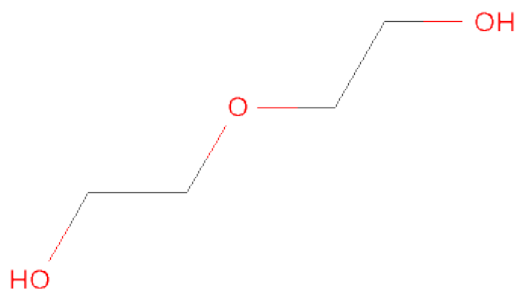
- Molecule 3 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	G	1	Total Ni 1 1	0	0
3	J	1	Total Ni 1 1	0	0
3	D	1	Total Ni 1 1	0	0
3	K	1	Total Ni 1 1	0	0
3	E	1	Total Ni 1 1	0	0
3	H	1	Total Ni 1 1	0	0
3	B	1	Total Ni 1 1	0	0
3	I	1	Total Ni 1 1	0	0
3	C	1	Total Ni 1 1	0	0
3	A	1	Total Ni 1 1	0	0
3	L	1	Total Ni 1 1	0	0
3	F	1	Total Ni 1 1	0	0

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Mg 1 1	0	0
4	K	1	Total Mg 1 1	0	0

- Molecule 5 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C₄H₁₀O₃).



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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	29	Total	O	0	0
			29	29		
6	D	19	Total	O	0	0
			19	19		
6	E	14	Total	O	0	0
			14	14		
6	B	40	Total	O	0	0
			40	40		
6	C	32	Total	O	0	0
			32	32		
6	F	15	Total	O	0	0
			15	15		
6	G	19	Total	O	0	0
			19	19		
6	H	14	Total	O	0	0
			14	14		
6	I	24	Total	O	0	0
			24	24		
6	J	29	Total	O	0	0
			29	29		
6	K	13	Total	O	0	0
			13	13		

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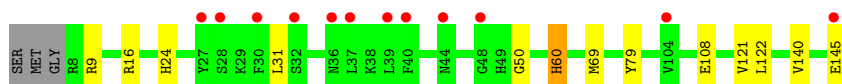
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	L	15	Total	O	0	0
			15	15		

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

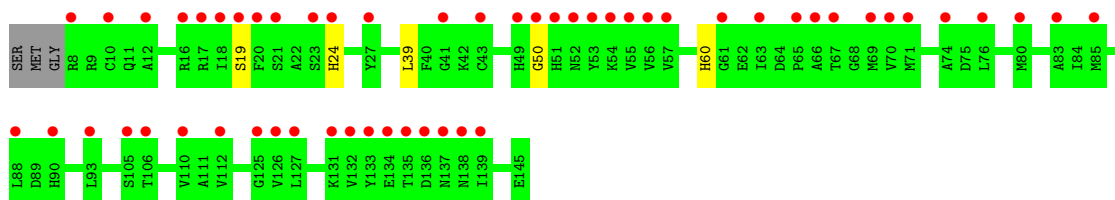
- Molecule 1: 6-pyruvoyl tetrahydrobiopterin synthase

Chain A: 



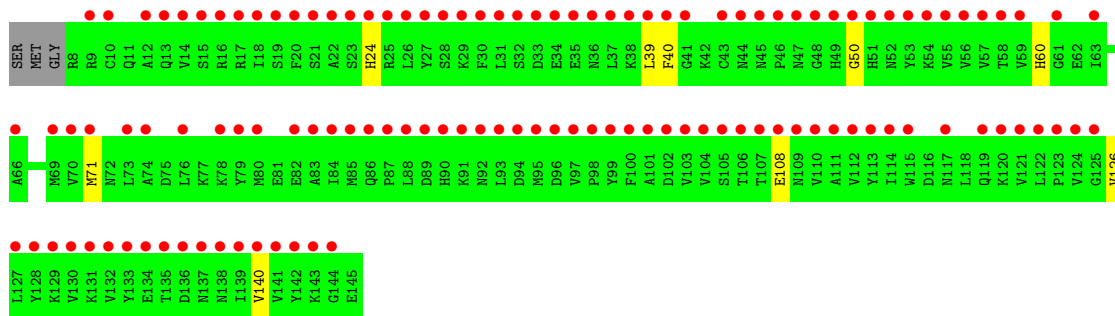
- Molecule 1: 6-pyruvoyl tetrahydrobiopterin synthase

Chain D: 



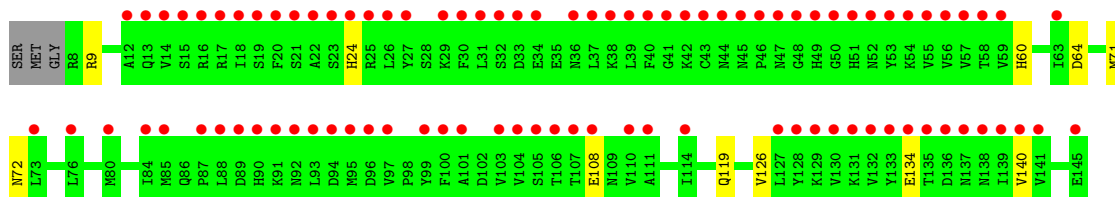
- Molecule 1: 6-pyruvoyl tetrahydrobiopterin synthase

Chain E: 



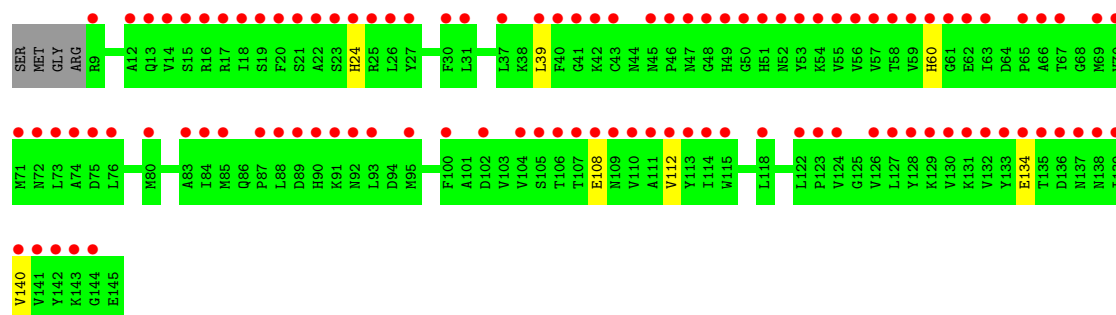
- Molecule 1: 6-pyruvoyl tetrahydrobiopterin synthase

Chain B: 



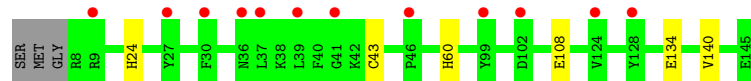
- Molecule 1: 6-pyruvoyl tetrahydrobiopterin synthase

Chain C:



- Molecule 1: 6-pyruvoyl tetrahydrobiopterin synthase

Chain F:



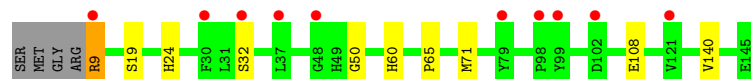
- Molecule 1: 6-pyruvoyl tetrahydrobiopterin synthase

Chain G:



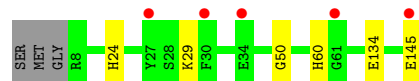
- Molecule 1: 6-pyruvoyl tetrahydrobiopterin synthase

Chain H:



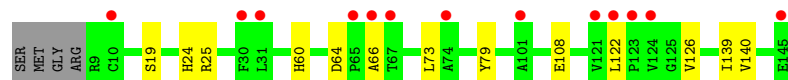
- Molecule 1: 6-pyruvoyl tetrahydrobiopterin synthase

Chain I:



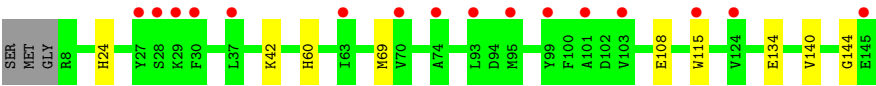
- Molecule 1: 6-pyruvoyl tetrahydrobiopterin synthase

Chain J:



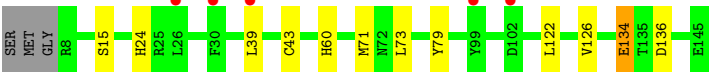
- Molecule 1: 6-pyruvoyl tetrahydrobiopterin synthase

Chain K:



● Molecule 1: 6-pyruvoyl tetrahydrobiopterin synthase

Chain L:



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	73.29Å 118.72Å 234.98Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.94 – 2.30 42.94 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.9 (42.94-2.30) 99.9 (42.94-2.30)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.08 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.5.0089	Depositor
R, R_{free}	0.206 , 0.246 0.207 , 0.248	Depositor DCC
R_{free} test set	4603 reflections (5.28%)	DCC
Wilson B-factor (Å ²)	41.9	Xtriage
Anisotropy	0.024	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 18.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	1 of 91835 reflections (0.001%)	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	13128	wwPDB-VP
Average B, all atoms (Å ²)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.76% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: NI, MG, PEG, EDO

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	0.86	0/1102	0.80	2/1497 (0.1%)
1	B	0.95	1/1119 (0.1%)	0.83	0/1517
1	C	0.86	2/1097 (0.2%)	0.76	0/1490
1	D	0.94	1/1128 (0.1%)	0.80	0/1531
1	E	0.83	0/1086	0.76	0/1478
1	F	0.80	2/1093 (0.2%)	0.73	0/1485
1	G	0.85	2/1062 (0.2%)	0.71	1/1444 (0.1%)
1	H	0.78	0/1067	0.69	1/1451 (0.1%)
1	I	0.84	1/1107 (0.1%)	0.75	0/1502
1	J	0.89	1/1085 (0.1%)	0.75	0/1474
1	K	0.81	1/1073 (0.1%)	0.72	0/1460
1	L	0.86	2/1102 (0.2%)	0.72	0/1499
All	All	0.86	13/13121 (0.1%)	0.75	4/17828 (0.0%)

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K	134	GLU	CD-OE2	7.63	1.34	1.25
1	G	134	GLU	CD-OE2	6.91	1.33	1.25
1	L	134	GLU	CD-OE2	6.50	1.32	1.25
1	B	134	GLU	CD-OE1	6.32	1.32	1.25
1	C	134	GLU	CD-OE2	5.60	1.31	1.25
1	C	112	VAL	CB-CG1	5.44	1.64	1.52
1	I	134	GLU	CD-OE2	5.31	1.31	1.25
1	F	134	GLU	CD-OE2	5.29	1.31	1.25
1	D	19	SER	CB-OG	-5.28	1.35	1.42
1	F	43	CYS	CB-SG	5.26	1.91	1.82
1	G	19	SER	CB-OG	-5.21	1.35	1.42
1	J	19	SER	CB-OG	-5.08	1.35	1.42
1	L	43	CYS	CB-SG	5.08	1.90	1.82

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	16	ARG	NE-CZ-NH2	-5.67	117.47	120.30
1	H	9	ARG	NE-CZ-NH1	5.22	122.91	120.30
1	G	25	ARG	NE-CZ-NH2	-5.21	117.69	120.30
1	A	9	ARG	NE-CZ-NH2	-5.00	117.80	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1080	0	1038	8	0
1	B	1093	0	1064	8	0
1	C	1071	0	1028	4	0
1	D	1099	0	1049	2	0
1	E	1064	0	996	7	0
1	F	1071	0	1022	1	0
1	G	1040	0	989	5	0
1	H	1045	0	973	3	0
1	I	1084	0	1035	1	0
1	J	1063	0	1018	5	0
1	K	1051	0	993	4	0
1	L	1079	0	1028	7	0
2	A	4	0	6	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
3	I	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	J	1	0	0	0	0
3	K	1	0	0	0	0
3	L	1	0	0	0	0
4	A	1	0	0	0	0
4	K	1	0	0	0	0
5	B	7	0	10	1	0
6	A	29	0	0	0	0
6	B	40	0	0	0	0
6	C	32	0	0	0	0
6	D	19	0	0	0	0
6	E	14	0	0	0	0
6	F	15	0	0	0	0
6	G	19	0	0	0	0
6	H	14	0	0	0	0
6	I	24	0	0	0	0
6	J	29	0	0	1	0
6	K	13	0	0	0	0
6	L	15	0	0	2	0
All	All	13128	0	12249	44	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 2.

All (44) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:71:MET:CE	1:E:126:VAL:HG11	2.05	0.86
1:J:25:ARG:HD3	6:J:161:HOH:O	1.90	0.72
1:E:71:MET:HE1	1:E:126:VAL:HG11	1.71	0.72
1:A:69:MET:HE1	1:D:39:LEU:HD11	1.74	0.69
1:G:30:PHE:O	1:G:31:LEU:HD23	1.95	0.66
1:B:72:ASN:ND2	1:C:39:LEU:HD12	2.15	0.61
1:E:71:MET:CE	1:E:126:VAL:CG1	2.80	0.60
1:J:64:ASP:OD1	1:J:66:ALA:HB3	2.04	0.58
1:A:79:TYR:CD2	1:A:122:LEU:HD23	2.40	0.56
1:K:69:MET:CE	1:L:39:LEU:HD11	2.37	0.54
1:L:134:GLU:OE2	6:L:155:HOH:O	2.18	0.54
1:B:71:MET:CE	1:B:126:VAL:HG11	2.39	0.52
1:E:50:GLY:HA3	1:H:50:GLY:HA3	1.92	0.51
1:B:119:GLN:OE1	1:B:119:GLN:HA	2.11	0.50
1:B:64:ASP:OD2	5:B:1:PEG:H22	2.11	0.49
1:H:9:ARG:HD3	1:H:65:PRO:HD3	1.95	0.49
1:G:123:PRO:HG2	1:G:126:VAL:HG21	1.94	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:108:GLU:HA	1:A:140:VAL:HG11	1.95	0.49
1:A:31:LEU:HD12	1:A:31:LEU:N	2.29	0.47
1:A:60:HIS:NE2	1:B:9:ARG:NH2	2.63	0.47
1:H:108:GLU:HA	1:H:140:VAL:HG11	1.97	0.46
1:F:108:GLU:HA	1:F:140:VAL:HG11	1.97	0.46
1:L:71:MET:CE	1:L:126:VAL:HG11	2.45	0.46
1:G:30:PHE:C	1:G:31:LEU:HD23	2.35	0.46
1:K:108:GLU:HA	1:K:140:VAL:HG11	1.98	0.45
1:E:108:GLU:HA	1:E:140:VAL:HG11	1.99	0.45
1:A:79:TYR:CD2	1:A:122:LEU:CD2	3.00	0.45
1:D:50:GLY:HA3	1:I:50:GLY:HA3	1.98	0.45
1:B:72:ASN:HD22	1:C:39:LEU:HD12	1.80	0.44
1:C:108:GLU:HA	1:C:140:VAL:HG11	1.99	0.44
1:B:108:GLU:HA	1:B:140:VAL:HG11	2.00	0.44
1:A:31:LEU:CD1	1:A:31:LEU:N	2.81	0.44
1:K:115:TRP:CZ2	1:K:144:GLY:HA3	2.53	0.44
1:L:136:ASP:OD2	6:L:149:HOH:O	2.21	0.43
1:E:39:LEU:HD23	1:E:40:PHE:CE2	2.54	0.43
1:J:108:GLU:HA	1:J:140:VAL:HG11	2.01	0.42
1:L:79:TYR:CD2	1:L:122:LEU:HD23	2.54	0.42
1:J:139:ILE:HB	1:L:15:SER:HB2	2.01	0.42
1:E:71:MET:HE3	1:E:126:VAL:CG1	2.49	0.42
1:K:69:MET:HE1	1:L:39:LEU:HD11	2.01	0.42
1:A:50:GLY:HA3	1:G:50:GLY:HA3	2.02	0.41
1:G:108:GLU:HA	1:G:140:VAL:HG11	2.03	0.41
1:B:72:ASN:ND2	1:C:39:LEU:CD1	2.83	0.41
1:J:79:TYR:CD2	1:J:122:LEU:HD23	2.56	0.40

There are no symmetry-related clashes.

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	136/141 (96%)	134 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	137/141 (97%)	135 (98%)	2 (2%)	0	100	100
1	C	136/141 (96%)	133 (98%)	3 (2%)	0	100	100
1	D	138/141 (98%)	136 (99%)	2 (1%)	0	100	100
1	E	136/141 (96%)	132 (97%)	4 (3%)	0	100	100
1	F	136/141 (96%)	132 (97%)	4 (3%)	0	100	100
1	G	134/141 (95%)	130 (97%)	4 (3%)	0	100	100
1	H	135/141 (96%)	132 (98%)	3 (2%)	0	100	100
1	I	136/141 (96%)	134 (98%)	2 (2%)	0	100	100
1	J	135/141 (96%)	132 (98%)	3 (2%)	0	100	100
1	K	136/141 (96%)	132 (97%)	4 (3%)	0	100	100
1	L	136/141 (96%)	134 (98%)	2 (2%)	0	100	100
All	All	1631/1692 (96%)	1596 (98%)	35 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	116/126 (92%)	112 (97%)	4 (3%)	49	64
1	B	117/126 (93%)	115 (98%)	2 (2%)	73	87
1	C	115/126 (91%)	113 (98%)	2 (2%)	73	87
1	D	118/126 (94%)	116 (98%)	2 (2%)	73	87
1	E	112/126 (89%)	110 (98%)	2 (2%)	71	86
1	F	113/126 (90%)	111 (98%)	2 (2%)	71	86
1	G	109/126 (86%)	106 (97%)	3 (3%)	56	73
1	H	106/126 (84%)	101 (95%)	5 (5%)	36	47
1	I	115/126 (91%)	111 (96%)	4 (4%)	48	63
1	J	113/126 (90%)	109 (96%)	4 (4%)	48	63
1	K	109/126 (86%)	106 (97%)	3 (3%)	56	73

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	L	117/126 (93%)	114 (97%)	3 (3%)	59	76
All	All	1360/1512 (90%)	1324 (97%)	36 (3%)	57	76

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	HIS
1	A	60	HIS
1	A	121	VAL
1	A	145	GLU
1	D	24	HIS
1	D	60	HIS
1	E	24	HIS
1	E	60	HIS
1	B	24	HIS
1	B	60	HIS
1	C	24	HIS
1	C	60	HIS
1	F	24	HIS
1	F	60	HIS
1	G	24	HIS
1	G	60	HIS
1	G	124	VAL
1	H	19	SER
1	H	24	HIS
1	H	32	SER
1	H	60	HIS
1	H	71	MET
1	I	24	HIS
1	I	29	LYS
1	I	60	HIS
1	I	145	GLU
1	J	24	HIS
1	J	60	HIS
1	J	73	LEU
1	J	126	VAL
1	K	24	HIS
1	K	42	LYS
1	K	60	HIS
1	L	24	HIS
1	L	60	HIS
1	L	73	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	60	HIS
1	E	60	HIS
1	B	60	HIS
1	C	60	HIS
1	F	60	HIS
1	H	60	HIS
1	I	60	HIS
1	J	60	HIS
1	K	60	HIS
1	L	60	HIS

5.3.3 RNA ⓘ

There are no RNA chains 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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 16 ligands modelled in this entry, 14 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	EDO	A	1	-	3,3,3	0.84	0	2,2,2	0.19	0
5	PEG	B	1	-	6,6,6	1.88	1 (16%)	5,5,5	0.66	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	EDO	A	1	-	-	0/1/1/1	0/0/0/0
5	PEG	B	1	-	-	0/4/4/4	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	1	PEG	O2-C3	3.07	1.55	1.42

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	138/141 (97%)	0.21	12 (8%) 10 16	8, 16, 29, 60	0
1	B	138/141 (97%)	3.26	91 (65%) 0 0	11, 15, 25, 37	0
1	C	137/141 (97%)	3.73	104 (75%) 0 0	7, 15, 26, 34	0
1	D	138/141 (97%)	1.80	55 (39%) 1 1	7, 15, 26, 38	0
1	E	138/141 (97%)	4.33	121 (87%) 0 0	9, 16, 27, 39	1 (0%)
1	F	138/141 (97%)	0.57	12 (8%) 10 16	6, 16, 25, 41	0
1	G	136/141 (96%)	0.27	3 (2%) 59 69	7, 15, 23, 28	1 (0%)
1	H	137/141 (97%)	0.46	10 (7%) 15 22	4, 16, 28, 34	0
1	I	138/141 (97%)	0.28	5 (3%) 41 51	3, 15, 27, 41	0
1	J	137/141 (97%)	0.39	13 (9%) 8 14	11, 15, 28, 38	0
1	K	138/141 (97%)	0.55	16 (11%) 5 9	4, 15, 30, 34	0
1	L	138/141 (97%)	0.37	5 (3%) 41 51	7, 15, 25, 37	1 (0%)
All	All	1651/1692 (97%)	1.35	447 (27%) 1 1	3, 15, 27, 60	3 (0%)

All (447) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	136	ASP	12.9
1	E	52	ASN	12.5
1	C	137	ASN	12.0
1	E	133	TYR	11.2
1	C	52	ASN	10.9
1	E	19	SER	10.8
1	E	90	HIS	10.7
1	E	135	THR	10.0
1	C	139	ILE	9.9
1	E	53	TYR	9.7
1	E	136	ASP	9.5

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Mol	Chain	Res	Type	RSRZ
1	B	43	CYS	9.4
1	E	50	GLY	9.2
1	C	133	TYR	9.1
1	E	48	GLY	9.0
1	C	135	THR	8.8
1	E	55	VAL	8.8
1	C	17	ARG	8.6
1	E	18	ILE	8.6
1	C	55	VAL	8.2
1	E	16	ARG	8.0
1	E	132	VAL	8.0
1	C	141	VAL	7.9
1	C	53	TYR	7.8
1	C	140	VAL	7.7
1	B	133	TYR	7.6
1	B	132	VAL	7.6
1	E	17	ARG	7.5
1	B	137	ASN	7.4
1	C	56	VAL	7.4
1	B	139	ILE	7.4
1	E	139	ILE	7.3
1	B	39	LEU	7.3
1	E	20	PHE	7.3
1	B	54	LYS	7.3
1	B	47	ASN	7.1
1	B	56	VAL	7.1
1	E	21	SER	7.0
1	B	17	ARG	7.0
1	E	95	MET	7.0
1	E	51	HIS	6.9
1	C	132	VAL	6.8
1	E	54	LYS	6.8
1	E	134	GLU	6.8
1	B	52	ASN	6.8
1	E	15	SER	6.7
1	E	39	LEU	6.7
1	B	40	PHE	6.6
1	B	138	ASN	6.6
1	E	138	ASN	6.6
1	C	138	ASN	6.6
1	B	48	GLY	6.6
1	B	50	GLY	6.6

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Mol	Chain	Res	Type	RSRZ
1	E	43	CYS	6.5
1	E	49	HIS	6.4
1	C	54	LYS	6.4
1	B	55	VAL	6.3
1	E	99	TYR	6.3
1	C	107	THR	6.3
1	C	42	LYS	6.3
1	E	56	VAL	6.2
1	E	140	VAL	6.2
1	B	140	VAL	6.2
1	E	106	THR	6.1
1	B	57	VAL	6.1
1	E	27	TYR	6.0
1	E	137	ASN	5.9
1	E	57	VAL	5.9
1	D	136	ASP	5.8
1	C	15	SER	5.8
1	C	18	ILE	5.8
1	C	20	PHE	5.8
1	C	90	HIS	5.7
1	E	22	ALA	5.7
1	C	16	ARG	5.6
1	C	110	VAL	5.6
1	A	39	LEU	5.6
1	B	31	LEU	5.6
1	C	130	VAL	5.6
1	E	88	LEU	5.6
1	B	136	ASP	5.6
1	B	33	ASP	5.5
1	C	142	TYR	5.5
1	B	15	SER	5.4
1	C	21	SER	5.4
1	C	14	VAL	5.4
1	B	34	GLU	5.4
1	C	71	MET	5.4
1	B	25[A]	ARG	5.4
1	B	19	SER	5.4
1	C	13	GLN	5.4
1	B	18	ILE	5.3
1	B	46	PRO	5.3
1	C	70	VAL	5.3
1	E	130	VAL	5.3

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Mol	Chain	Res	Type	RSRZ
1	B	130	VAL	5.2
1	C	69	MET	5.2
1	E	141	VAL	5.2
1	E	47	ASN	5.2
1	B	53	TYR	5.2
1	C	131	LYS	5.2
1	C	19	SER	5.2
1	B	58	THR	5.1
1	C	51	HIS	5.1
1	D	137	ASN	5.1
1	E	14	VAL	5.0
1	E	124	VAL	5.0
1	C	40	PHE	5.0
1	C	24	HIS	5.0
1	B	32	SER	5.0
1	E	103	VAL	5.0
1	E	40	PHE	5.0
1	E	110	VAL	4.9
1	B	135	THR	4.9
1	B	95	MET	4.9
1	C	108	GLU	4.9
1	C	105	SER	4.8
1	C	88	LEU	4.8
1	E	107	THR	4.7
1	B	23	SER	4.7
1	E	71	MET	4.7
1	B	30	PHE	4.7
1	D	52	ASN	4.7
1	B	49	HIS	4.7
1	B	26	LEU	4.7
1	E	104	VAL	4.7
1	B	141	VAL	4.7
1	C	57	VAL	4.7
1	E	113	TYR	4.7
1	B	41	GLY	4.6
1	E	105	SER	4.6
1	B	16	ARG	4.6
1	E	122	LEU	4.6
1	C	43	CYS	4.6
1	E	83	ALA	4.6
1	B	73	LEU	4.6
1	B	131	LYS	4.6

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Mol	Chain	Res	Type	RSRZ
1	E	84	ILE	4.5
1	D	53	TYR	4.5
1	B	110	VAL	4.5
1	E	123	PRO	4.5
1	B	22	ALA	4.5
1	C	23	SER	4.4
1	C	58	THR	4.4
1	B	21	SER	4.4
1	E	24	HIS	4.4
1	B	20	PHE	4.4
1	E	131	LYS	4.4
1	B	45	ASN	4.4
1	E	80	MET	4.3
1	C	74	ALA	4.3
1	C	128	TYR	4.3
1	E	111	ALA	4.3
1	B	24	HIS	4.2
1	E	98	PRO	4.2
1	E	33	ASP	4.2
1	C	112	VAL	4.2
1	J	10	CYS	4.2
1	C	134	GLU	4.2
1	C	84	ILE	4.2
1	B	38	LYS	4.2
1	E	92	ASN	4.2
1	E	100	PHE	4.2
1	C	41	GLY	4.1
1	E	143	LYS	4.1
1	E	102	ASP	4.1
1	I	30	PHE	4.1
1	C	22	ALA	4.1
1	E	87	PRO	4.0
1	C	111	ALA	4.0
1	C	50	GLY	4.0
1	B	51	HIS	4.0
1	C	26	LEU	4.0
1	E	89	ASP	4.0
1	E	96	ASP	4.0
1	C	73	LEU	3.9
1	E	97	VAL	3.9
1	C	129	LYS	3.9
1	C	85	MET	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	30	PHE	3.9
1	E	28	SER	3.9
1	C	75	ASP	3.9
1	E	37	LEU	3.9
1	C	104	VAL	3.8
1	D	67	THR	3.8
1	D	54	LYS	3.8
1	D	24	HIS	3.8
1	D	135	THR	3.8
1	B	107	THR	3.8
1	E	121	VAL	3.8
1	C	106	THR	3.8
1	D	20	PHE	3.8
1	E	115	TRP	3.8
1	D	70	VAL	3.8
1	E	117	ASN	3.8
1	C	109	ASN	3.8
1	E	31	LEU	3.8
1	C	27	TYR	3.8
1	B	36	ASN	3.7
1	B	14	VAL	3.7
1	C	143	LYS	3.7
1	H	121	VAL	3.7
1	B	37	LEU	3.7
1	E	128	TYR	3.7
1	E	112	VAL	3.7
1	D	85	MET	3.7
1	B	111	ALA	3.6
1	E	26	LEU	3.6
1	B	88	LEU	3.6
1	C	144	GLY	3.6
1	F	41	GLY	3.6
1	K	27	TYR	3.6
1	D	139	ILE	3.6
1	C	114	ILE	3.6
1	E	109	ASN	3.6
1	C	12	ALA	3.6
1	E	93	LEU	3.6
1	B	100	PHE	3.6
1	C	83	ALA	3.5
1	B	106	THR	3.5
1	B	27	TYR	3.5

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Mol	Chain	Res	Type	RSRZ
1	E	23	SER	3.5
1	E	46	PRO	3.5
1	K	124	VAL	3.5
1	C	9	ARG	3.5
1	C	49	HIS	3.5
1	D	63	ILE	3.4
1	E	120	LYS	3.4
1	D	21	SER	3.4
1	B	93	LEU	3.4
1	B	128	TYR	3.4
1	B	134	GLU	3.4
1	A	28	SER	3.4
1	B	96	ASP	3.4
1	C	63	ILE	3.4
1	C	113	TYR	3.3
1	E	70	VAL	3.3
1	C	95	MET	3.3
1	C	48	GLY	3.3
1	D	51	HIS	3.3
1	B	29	LYS	3.3
1	E	41	GLY	3.3
1	B	87	PRO	3.3
1	B	80	MET	3.3
1	K	63	ILE	3.3
1	E	101	ALA	3.3
1	D	133	TYR	3.2
1	E	12	ALA	3.2
1	E	94	ASP	3.2
1	C	61	GLY	3.2
1	E	34	GLU	3.2
1	E	142	TYR	3.2
1	C	126	VAL	3.2
1	D	69	MET	3.2
1	E	69	MET	3.2
1	F	99	TYR	3.2
1	D	8	ARG	3.2
1	E	79	TYR	3.1
1	C	60	HIS	3.1
1	D	23	SER	3.1
1	B	59	VAL	3.1
1	E	45	ASN	3.1
1	B	108	GLU	3.1

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Mol	Chain	Res	Type	RSRZ
1	E	85	MET	3.1
1	K	29	LYS	3.1
1	F	124	VAL	3.1
1	C	115	TRP	3.1
1	B	42	LYS	3.1
1	E	127	LEU	3.0
1	K	99	TYR	3.0
1	C	59	VAL	3.0
1	G	41	GLY	3.0
1	J	121	VAL	3.0
1	E	44	ASN	3.0
1	B	90	HIS	3.0
1	E	59	VAL	3.0
1	B	76	LEU	3.0
1	C	37	LEU	3.0
1	C	93	LEU	3.0
1	D	18	ILE	3.0
1	C	89	ASP	3.0
1	F	30	PHE	3.0
1	H	30	PHE	3.0
1	C	45	ASN	3.0
1	C	47	ASN	3.0
1	D	90	HIS	2.9
1	E	32	SER	2.9
1	B	84	ILE	2.9
1	E	13	GLN	2.9
1	E	58	THR	2.9
1	L	99	TYR	2.9
1	L	102	ASP	2.9
1	D	132	VAL	2.9
1	B	97	VAL	2.9
1	D	17	ARG	2.9
1	D	105	SER	2.9
1	D	74	ALA	2.9
1	A	27	TYR	2.9
1	E	114	ILE	2.8
1	J	123	PRO	2.8
1	D	19	SER	2.8
1	D	61	GLY	2.8
1	F	36	ASN	2.8
1	C	92	ASN	2.8
1	B	13	GLN	2.8

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Mol	Chain	Res	Type	RSRZ
1	E	25	ARG	2.8
1	D	80	MET	2.8
1	H	98	PRO	2.8
1	A	145	GLU	2.8
1	K	74	ALA	2.8
1	E	38	LYS	2.8
1	L	39	LEU	2.8
1	E	129	LYS	2.7
1	D	56	VAL	2.7
1	E	30	PHE	2.7
1	B	101	ALA	2.7
1	C	80	MET	2.7
1	B	129	LYS	2.7
1	F	27	TYR	2.7
1	C	25	ARG	2.7
1	A	104	VAL	2.7
1	D	88	LEU	2.7
1	B	92	ASN	2.7
1	A	40	PHE	2.7
1	B	103	VAL	2.6
1	K	28	SER	2.6
1	D	27	TYR	2.6
1	E	10	CYS	2.6
1	C	127	LEU	2.6
1	D	16	ARG	2.6
1	D	71	MET	2.6
1	E	125	GLY	2.6
1	H	32	SER	2.6
1	B	114	ILE	2.6
1	E	9	ARG	2.6
1	C	87	PRO	2.6
1	G	72	ASN	2.6
1	D	126	VAL	2.6
1	C	76	LEU	2.6
1	B	44	ASN	2.6
1	B	85	MET	2.6
1	E	35	GLU	2.6
1	D	76	LEU	2.6
1	D	12	ALA	2.5
1	C	39	LEU	2.5
1	E	119	GLN	2.5
1	D	66	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	K	101	ALA	2.5
1	D	10	CYS	2.5
1	H	48	GLY	2.5
1	E	91	LYS	2.5
1	B	99	TYR	2.5
1	K	37	LEU	2.5
1	C	124	VAL	2.5
1	H	9	ARG	2.5
1	H	79	TYR	2.5
1	J	65	PRO	2.5
1	J	124	VAL	2.5
1	A	37	LEU	2.4
1	C	66	ALA	2.4
1	C	65	PRO	2.4
1	D	55	VAL	2.4
1	G	124	VAL	2.4
1	J	145	GLU	2.4
1	C	118	LEU	2.4
1	D	65	PRO	2.4
1	B	89	ASP	2.4
1	A	44	ASN	2.4
1	D	93	LEU	2.4
1	B	127	LEU	2.4
1	K	145	GLU	2.4
1	J	66	ALA	2.4
1	A	32	SER	2.4
1	D	127	LEU	2.3
1	C	62	GLU	2.3
1	C	30	PHE	2.3
1	I	145	GLU	2.3
1	J	74	ALA	2.3
1	B	91	LYS	2.3
1	F	9	ARG	2.3
1	K	93	LEU	2.3
1	D	110	VAL	2.3
1	D	112	VAL	2.3
1	B	12	ALA	2.3
1	B	104	VAL	2.3
1	J	101	ALA	2.3
1	F	46	PRO	2.3
1	H	102	ASP	2.3
1	E	29	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	E	61	GLY	2.3
1	E	144	GLY	2.3
1	J	30	PHE	2.3
1	C	31	LEU	2.3
1	J	122	LEU	2.3
1	B	94	ASP	2.3
1	J	67	THR	2.3
1	E	82	GLU	2.3
1	E	78	LYS	2.3
1	D	106	THR	2.3
1	C	123	PRO	2.3
1	F	102	ASP	2.2
1	D	138	ASN	2.2
1	K	103	VAL	2.2
1	C	67	THR	2.2
1	I	61	GLY	2.2
1	E	66	ALA	2.2
1	J	31	LEU	2.2
1	D	49	HIS	2.2
1	C	91	LYS	2.2
1	E	74	ALA	2.2
1	K	95	MET	2.2
1	H	37	LEU	2.1
1	B	145	GLU	2.1
1	A	48	GLY	2.1
1	E	63	ILE	2.1
1	L	30	PHE	2.1
1	A	36	ASN	2.1
1	E	73	LEU	2.1
1	E	86	GLN	2.1
1	F	37	LEU	2.1
1	E	76	LEU	2.1
1	C	122	LEU	2.1
1	F	39	LEU	2.1
1	D	41	GLY	2.1
1	E	36	ASN	2.1
1	C	46	PRO	2.1
1	C	72	ASN	2.1
1	F	128	TYR	2.1
1	H	99	TYR	2.1
1	B	105	SER	2.1
1	C	100	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	125	GLY	2.1
1	D	57	VAL	2.1
1	K	115	TRP	2.1
1	B	63	ILE	2.1
1	D	83	ALA	2.1
1	D	50	GLY	2.0
1	E	108	GLU	2.0
1	I	34	GLU	2.0
1	D	131	LYS	2.0
1	I	27	TYR	2.0
1	D	134	GLU	2.0
1	K	30	PHE	2.0
1	C	102[A]	ASP	2.0
1	L	26	LEU	2.0
1	K	70	VAL	2.0
1	D	43	CYS	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
4	MG	A	2	1/1	0.26	2.33	56,56,56,56	0
5	PEG	B	1	7/7	0.21	1.20	41,44,63,67	0
2	EDO	A	1	4/4	0.24	0.86	63,73,85,86	0
3	NI	I	146	1/1	0.04	-1.29	31,31,31,31	0
4	MG	K	1	1/1	0.08	-1.95	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	NI	L	146	1/1	0.04	-2.16	41,41,41,41	0
3	NI	J	146	1/1	0.06	-2.73	29,29,29,29	0
3	NI	F	146	1/1	0.04	-2.74	40,40,40,40	0
3	NI	D	4	1/1	0.03	-2.95	29,29,29,29	0
3	NI	G	146	1/1	0.03	-3.13	35,35,35,35	0
3	NI	K	146	1/1	0.03	-3.19	33,33,33,33	0
3	NI	H	146	1/1	0.03	-4.03	36,36,36,36	0
3	NI	A	146	1/1	0.03	-4.09	33,33,33,33	0
3	NI	E	146	1/1	0.04	-4.89	35,35,35,35	0
3	NI	C	3	1/1	0.04	-5.35	29,29,29,29	0
3	NI	B	2	1/1	0.04	-6.69	31,31,31,31	0

6.5 Other polymers ⓘ

There are no such residues in this entry.