



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2026 – 05:47 PM UTC

PDB ID : 6S9M / pdb_00006s9m
Title : Designed Armadillo Repeat protein Lock2 fused to target peptide KRKRKAK-ITW
Authors : Ernst, P.; Zosel, F.; Reichen, C.; Schuler, B.; Pluckthun, A.
Deposited on : 2019-07-15
Resolution : 2.00 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

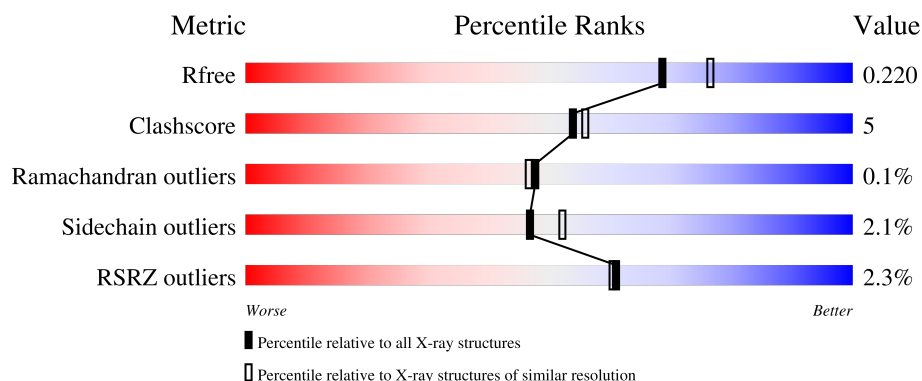
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	302	2% 89% 8% ..
1	B	302	91% 7% ..
1	C	302	6% 91% 7% ..
1	D	302	% 89% 8% ..
1	E	302	% 90% 9% .

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Mol	Chain	Length	Quality of chain
1	F	302	4% 86% 12% ..

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 14653 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 Lock2_KRK RKAKITW.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	300	Total	C	N	O	S	0	4	0
			2251	1400	395	454	2			
1	B	299	Total	C	N	O	S	0	3	0
			2238	1393	394	449	2			
1	C	300	Total	C	N	O	S	0	1	0
			2215	1378	389	446	2			
1	D	298	Total	C	N	O	S	0	5	0
			2244	1394	392	456	2			
1	E	301	Total	C	N	O	S	0	5	0
			2256	1401	399	454	2			
1	F	298	Total	C	N	O	S	0	7	0
			2238	1390	394	452	2			

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

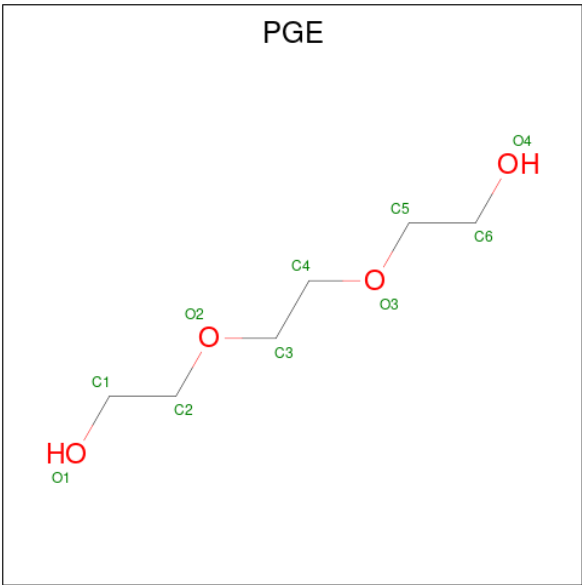
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	6	Total	Ca	0	0
			6	6		
2	B	6	Total	Ca	0	0
			6	6		
2	D	3	Total	Ca	0	0
			3	3		
2	F	3	Total	Ca	0	0
			3	3		

- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



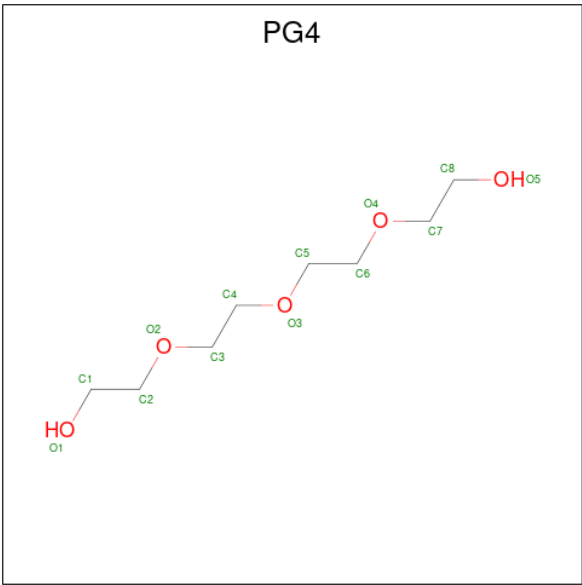
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	D	1	Total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

- Molecule 4 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: C₆H₁₄O₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	C	1	Total	C	O	0	0
			10	6	4		
4	D	1	Total	C	O	0	0
			10	6	4		
4	E	1	Total	C	O	0	0
			10	6	4		

- Molecule 5 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: C₈H₁₈O₅).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	D	1	Total	C	O	0	0
			13	8	5		

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

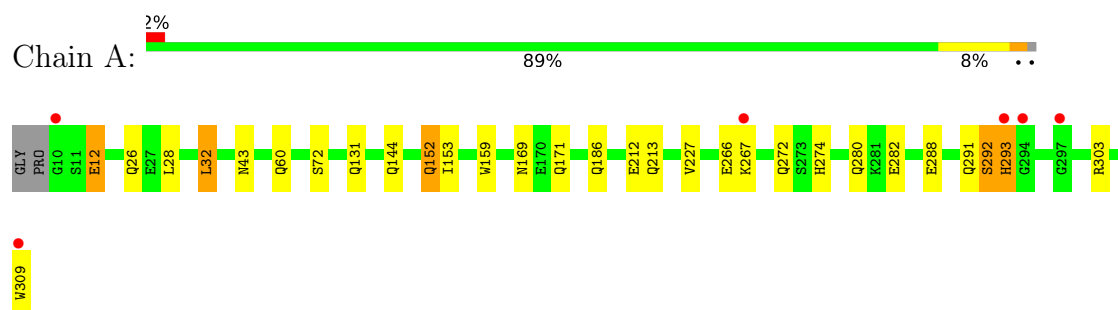
- Molecule 6 is water.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	203	Total	O		0	0
			203	203			
6	B	198	Total	O		0	0
			198	198			
6	C	123	Total	O		0	0
			123	123			
6	D	204	Total	O		0	0
			204	204			
6	E	185	Total	O		0	0
			185	185			
6	F	159	Total	O		0	0
			159	159			

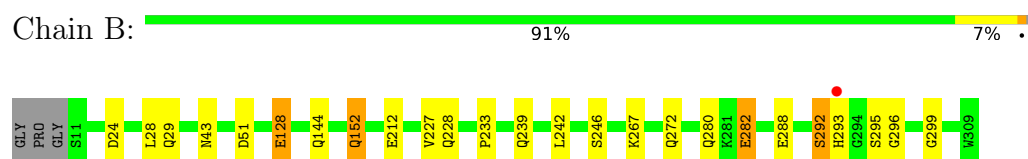
3 Residue-property plots [i](#)

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.

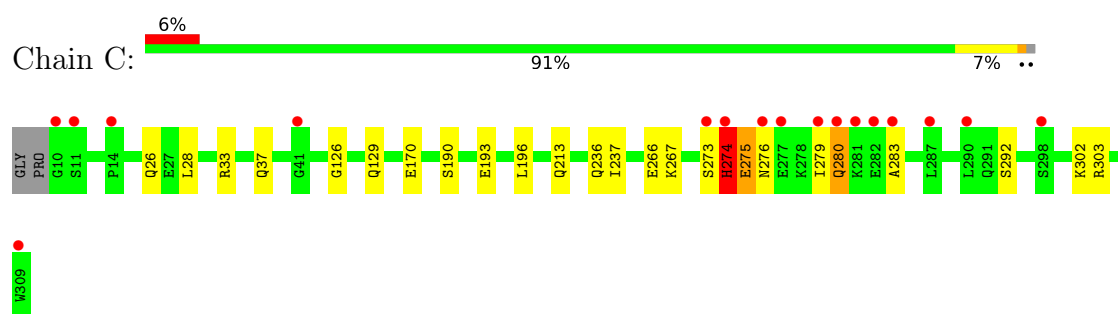
- Molecule 1: Lock2_KRK RKAKITW



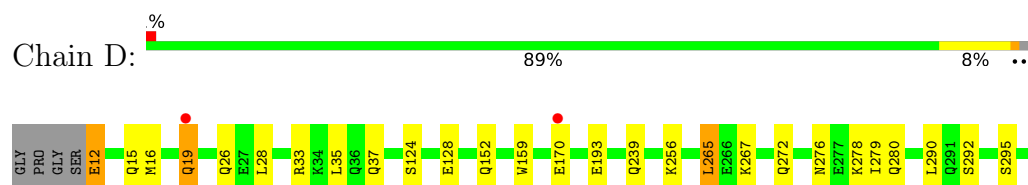
- Molecule 1: Lock2_KRK RKAKITW



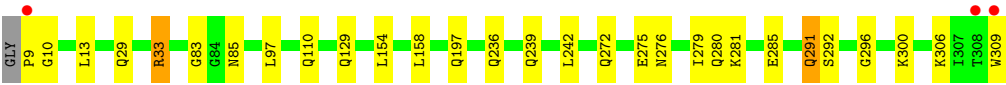
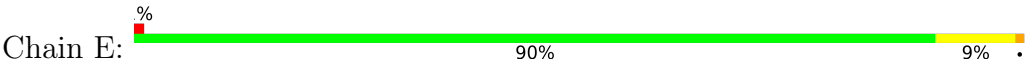
- Molecule 1: Lock2_KRK RKAKITW



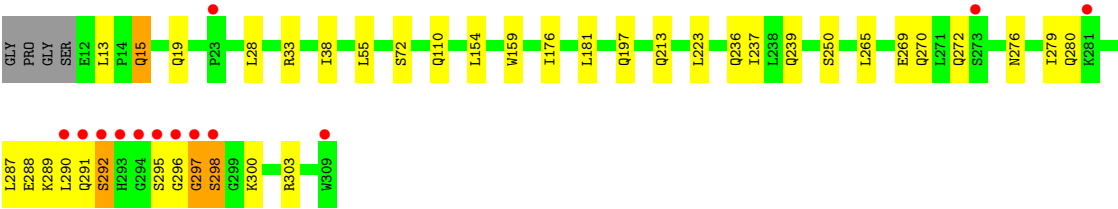
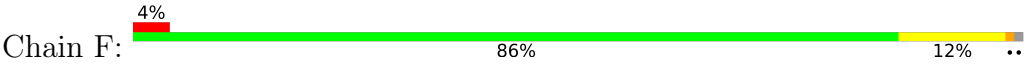
- Molecule 1: Lock2_KRK RKAKITW



- Molecule 1: Lock2_KRK RKAKITW



• Molecule 1: Lock2_KRK RKAKITW



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	54.85Å 85.47Å 193.97Å 90.00° 96.32° 90.00°	Depositor
Resolution (Å)	48.20 – 2.00 48.20 – 2.00	Depositor EDS
% Data completeness (in resolution range)	98.0 (48.20-2.00) 98.0 (48.20-2.00)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.37 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.8.0189	Depositor
R, R_{free}	0.177 , 0.213 0.188 , 0.220	Depositor DCC
R_{free} test set	5904 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	28.6	Xtriage
Anisotropy	0.365	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 39.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.002 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	14653	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.58% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: EDO, CA, PG4, PGE

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.29	2/2273 (0.1%)	1.07	6/3081 (0.2%)
1	B	1.29	3/2260 (0.1%)	1.07	3/3064 (0.1%)
1	C	1.20	4/2237 (0.2%)	1.07	4/3035 (0.1%)
1	D	1.29	2/2266 (0.1%)	1.04	1/3074 (0.0%)
1	E	1.29	3/2279 (0.1%)	1.06	1/3091 (0.0%)
1	F	1.34	6/2260 (0.3%)	1.11	4/3065 (0.1%)
All	All	1.28	20/13575 (0.1%)	1.07	19/18410 (0.1%)

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	F	0	1

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	299	GLY	CA-C	6.76	1.57	1.52
1	F	295	SER	CA-C	6.74	1.60	1.52
1	C	213	GLN	CG-CD	-6.31	1.36	1.52
1	F	19	GLN	C-O	5.96	1.31	1.24
1	C	170	GLU	CG-CD	5.71	1.66	1.52
1	C	274	HIS	CA-CB	5.69	1.63	1.53
1	F	181	LEU	N-CA	5.66	1.51	1.46
1	B	212	GLU	CG-CD	5.63	1.66	1.52
1	E	275	GLU	N-CA	5.59	1.53	1.46
1	E	97	LEU	N-CA	5.55	1.51	1.46
1	F	55	LEU	N-CA	5.46	1.52	1.46
1	D	12	GLU	N-CA	5.44	1.56	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	152	GLN	CD-OE1	5.33	1.33	1.23
1	E	83	GLY	N-CA	5.31	1.51	1.45
1	F	223	LEU	N-CA	5.30	1.51	1.46
1	C	273	SER	C-O	5.26	1.30	1.23
1	B	246	SER	N-CA	-5.22	1.40	1.46
1	A	171	GLN	N-CA	-5.21	1.40	1.46
1	F	176	ILE	N-CA	5.18	1.52	1.46
1	A	153	ILE	CA-CB	5.05	1.60	1.54

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	170	GLU	CB-CG-CD	9.47	128.70	112.60
1	F	213	GLN	CA-CB-CG	-9.28	95.54	114.10
1	C	213	GLN	CA-CB-CG	-9.07	95.96	114.10
1	C	33	ARG	NE-CZ-NH2	7.57	126.02	119.20
1	F	270	GLN	CA-CB-CG	7.00	128.10	114.10
1	F	295	SER	N-CA-C	6.81	119.68	108.92
1	F	15	GLN	CB-CG-CD	-6.80	101.04	112.60
1	A	186	GLN	CB-CG-CD	6.52	123.68	112.60
1	E	291	GLN	CA-CB-CG	-6.49	101.12	114.10
1	A	293	HIS	CA-C-O	-6.22	113.89	120.80
1	C	274	HIS	CB-CA-C	6.14	122.64	110.42
1	B	212	GLU	CB-CG-CD	6.04	122.86	112.60
1	A	12	GLU	N-CA-C	5.48	119.81	113.18
1	D	19	GLN	CA-CB-CG	5.47	125.04	114.10
1	B	295	SER	CA-CB-OG	5.45	121.99	111.10
1	A	293	HIS	N-CA-C	-5.39	100.92	109.76
1	A	212	GLU	CB-CG-CD	5.12	121.30	112.60
1	B	43	ASN	N-CA-C	5.04	117.67	111.82
1	A	43	ASN	N-CA-C	5.03	117.50	111.71

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	F	297[A]	GLY	Peptide

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	2251	0	2287	30	0
1	B	2238	0	2281	22	0
1	C	2215	0	2252	16	0
1	D	2244	0	2268	24	1
1	E	2256	0	2288	31	0
1	F	2238	0	2268	26	1
2	A	6	0	0	0	0
2	B	6	0	0	0	0
2	D	3	0	0	1	0
2	F	3	0	0	0	0
3	A	16	0	24	1	0
3	B	16	0	24	0	0
3	D	8	0	12	1	0
3	E	8	0	12	0	0
3	F	4	0	6	0	0
4	C	10	0	14	1	0
4	D	10	0	14	0	0
4	E	10	0	14	5	0
5	D	13	0	18	4	0
5	E	26	0	36	2	0
6	A	203	0	0	7	1
6	B	198	0	0	10	0
6	C	123	0	0	4	0
6	D	204	0	0	4	4
6	E	185	0	0	5	3
6	F	159	0	0	5	6
All	All	14653	0	13818	135	8

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 5.

All (135) 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:B:152:GLN:OE1	6:B:501:HOH:O	1.64	1.14

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:152:GLN:OE1	6:A:501:HOH:O	1.73	1.06
2:D:401:CA:CA	6:D:501:HOH:O	1.35	1.04
1:F:72:SER:HB3	6:F:516:HOH:O	1.80	0.81
1:A:213:GLN:CD	6:A:502:HOH:O	2.27	0.77
1:C:274:HIS:O	1:C:275:GLU:HG3	1.85	0.77
1:A:309:TRP:HA	4:E:405:PGE:H2	1.68	0.76
1:A:309:TRP:HA	4:E:405:PGE:C2	2.16	0.75
1:E:300:LYS:H	1:F:297[A]:GLY:HA3	1.49	0.75
1:A:169:ASN:O	6:A:502:HOH:O	2.05	0.75
1:D:15:GLN:O	1:D:19:GLN:HG2	1.90	0.72
1:F:159:TRP:CD2	1:F:303[A]:ARG:HD3	2.26	0.71
1:D:193:GLU:OE1	6:D:501:HOH:O	2.08	0.71
1:B:128:GLU:H	1:B:128:GLU:CD	1.98	0.71
1:D:170[C]:GLU:OE1	1:D:170[C]:GLU:C	2.34	0.70
1:A:309:TRP:CZ2	6:A:503:HOH:O	2.44	0.69
1:E:197:GLN:NE2	1:E:236[B]:GLN:HE21	1.92	0.68
1:C:196:LEU:HD13	6:C:510:HOH:O	1.93	0.68
1:B:144[B]:GLN:OE1	6:B:502:HOH:O	2.12	0.67
1:F:289:LYS:HE3	1:F:296[B]:GLY:O	1.95	0.65
1:C:126:GLY:H	1:C:129:GLN:HE21	1.44	0.65
1:D:16:MET:CE	1:D:35:LEU:CD2	2.75	0.65
1:D:33:ARG:HH12	1:D:37:GLN:HE21	1.45	0.65
1:C:276:ASN:HB3	1:C:279:ILE:HD12	1.78	0.64
1:D:16:MET:HE2	1:D:35:LEU:CD2	2.28	0.63
1:D:16:MET:HE2	1:D:35:LEU:HD21	1.81	0.63
1:E:33[A]:ARG:NH2	1:E:309:TRP:O	2.32	0.62
1:E:197:GLN:HE21	1:E:236[B]:GLN:NE2	1.98	0.62
1:F:289:LYS:HE2	1:F:297[B]:GLY:HA2	1.81	0.62
1:C:274:HIS:O	1:C:275:GLU:CG	2.49	0.61
1:A:26:GLN:HE21	1:E:236[A]:GLN:HE21	1.49	0.60
1:A:159:TRP:CD2	1:A:303[B]:ARG:HD3	2.35	0.60
1:E:300:LYS:HB2	1:F:297[A]:GLY:HA2	1.82	0.60
1:C:126:GLY:H	1:C:129:GLN:NE2	1.98	0.60
1:D:16:MET:HE3	1:D:35:LEU:HG	1.84	0.60
1:E:281:LYS:NZ	1:E:285:GLU:OE1	2.35	0.59
1:B:242:LEU:HB3	1:B:282:GLU:HG2	1.83	0.59
1:E:197:GLN:NE2	1:E:236[B]:GLN:NE2	2.50	0.59
1:F:110:GLN:NE2	6:F:501:HOH:O	2.10	0.58
1:B:293:HIS:HB3	5:D:406:PG4:C7	2.32	0.58
1:E:300:LYS:H	1:F:297[A]:GLY:CA	2.18	0.57
1:A:26:GLN:HE21	1:E:236[A]:GLN:NE2	2.02	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:228:GLN:OE1	6:B:503:HOH:O	2.17	0.57
1:C:275:GLU:C	1:C:280:GLN:HE22	2.13	0.56
1:D:128[B]:GLU:H	1:D:128[B]:GLU:CD	2.13	0.56
1:F:197:GLN:OE1	1:F:236[B]:GLN:NE2	2.32	0.56
1:E:239:GLN:HG2	6:E:570:HOH:O	2.06	0.55
1:B:293:HIS:HB3	5:D:406:PG4:H72	1.89	0.54
1:D:33:ARG:HH12	1:D:37:GLN:NE2	2.04	0.54
1:E:306:LYS:HB2	4:E:405:PGE:H12	1.90	0.54
1:B:29:GLN:HG2	1:C:236:GLN:HE22	1.71	0.53
1:B:292:SER:OG	6:B:504:HOH:O	2.19	0.53
1:D:16:MET:CE	1:D:35:LEU:HD23	2.38	0.53
1:A:152:GLN:HG3	6:E:501:HOH:O	2.08	0.52
6:B:588:HOH:O	1:C:276:ASN:HB2	2.09	0.52
1:D:256:LYS:HE2	6:D:654:HOH:O	2.10	0.52
1:E:197:GLN:HE21	1:E:236[B]:GLN:HE21	1.55	0.51
1:F:13:LEU:HD21	1:F:38:ILE:HD13	1.93	0.51
1:C:193:GLU:HG3	1:C:237:ILE:HD11	1.93	0.51
1:A:213:GLN:NE2	6:A:502:HOH:O	2.43	0.51
1:F:154:LEU:C	1:F:154:LEU:HD23	2.37	0.50
1:D:124:SER:O	5:D:406:PG4:H81	2.12	0.50
1:B:51:ASP:OD2	6:B:505:HOH:O	2.20	0.49
1:B:280:GLN:NE2	6:B:508:HOH:O	2.43	0.49
1:D:295:SER:OG	3:D:404:EDO:H11	2.11	0.49
1:E:296:GLY:HA3	1:F:300:LYS:O	2.13	0.49
1:A:26:GLN:OE1	1:E:239:GLN:OE1	2.30	0.48
1:F:303[A]:ARG:NH2	6:F:504:HOH:O	2.46	0.48
1:E:154:LEU:C	1:E:154:LEU:HD23	2.38	0.48
1:B:296:GLY:HA2	6:B:605:HOH:O	2.14	0.48
1:E:85:ASN:HD22	5:E:403:PG4:H12	1.78	0.48
1:B:227:VAL:CG1	1:B:267[A]:LYS:HE3	2.44	0.48
1:D:28:LEU:C	1:D:28:LEU:HD23	2.39	0.47
1:F:265:LEU:CD2	1:F:290:LEU:HD13	2.45	0.47
1:A:309:TRP:CH2	6:A:503:HOH:O	2.67	0.47
1:F:287:LEU:O	1:F:291:GLN:HG2	2.15	0.47
1:F:297[A]:GLY:O	1:F:298[A]:SER:C	2.58	0.47
1:B:267[B]:LYS:CE	6:B:515:HOH:O	2.63	0.47
1:F:276:ASN:HB3	1:F:279:ILE:HD12	1.96	0.47
1:B:288:GLU:O	1:B:292:SER:HB3	2.15	0.47
1:A:288:GLU:O	1:A:292:SER:HB3	2.15	0.47
1:F:250:SER:HB3	1:F:296[A]:GLY:HA2	1.97	0.46
1:E:110:GLN:NE2	6:E:501:HOH:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:26:GLN:NE2	6:D:502:HOH:O	2.25	0.46
1:A:267[C]:LYS:CD	1:A:267[C]:LYS:N	2.79	0.45
1:B:272:GLN:O	1:B:280:GLN:HG3	2.16	0.45
1:E:306:LYS:HB2	4:E:405:PGE:C1	2.46	0.45
1:A:26:GLN:HE22	1:E:239:GLN:CD	2.25	0.45
1:A:272:GLN:O	1:A:280:GLN:HG2	2.17	0.45
1:A:32:LEU:HD13	1:A:72:SER:HB2	1.99	0.45
1:F:265:LEU:HD13	1:F:287:LEU:HD21	1.98	0.45
1:B:267[C]:LYS:NZ	6:B:510:HOH:O	2.44	0.45
1:F:28:LEU:C	1:F:28:LEU:HD23	2.42	0.45
1:A:309:TRP:HA	4:E:405:PGE:H22	1.99	0.45
1:A:152:GLN:NE2	6:E:501:HOH:O	2.50	0.44
1:A:267[B]:LYS:H	1:A:267[B]:LYS:HG2	1.48	0.44
1:A:26:GLN:HG3	1:E:236[A]:GLN:NE2	2.32	0.44
1:F:269:GLU:HG3	1:F:287:LEU:HD11	2.00	0.44
1:A:131:GLN:HE22	3:A:406:EDO:H21	1.83	0.44
1:D:239:GLN:OE1	1:D:278:LYS:HG3	2.18	0.44
1:D:170[C]:GLU:OE1	1:D:170[C]:GLU:O	2.35	0.44
1:D:159:TRP:CE2	1:D:303[B]:ARG:HD2	2.53	0.43
1:B:152:GLN:HG3	6:C:501:HOH:O	2.16	0.43
1:D:124:SER:O	5:D:406:PG4:C8	2.67	0.43
1:E:272:GLN:O	1:E:280:GLN:HG2	2.18	0.43
1:F:237:ILE:HD13	6:F:510:HOH:O	2.18	0.43
1:A:266[A]:GLU:HB2	1:B:233:PRO:HD3	2.01	0.43
1:A:274:HIS:O	1:A:280:GLN:HG3	2.19	0.43
1:A:144:GLN:NE2	6:A:520:HOH:O	2.52	0.43
1:E:9:PRO:O	1:E:13:LEU:CD1	2.66	0.43
1:A:26:GLN:NE2	1:E:239:GLN:OE1	2.52	0.43
1:C:283:ALA:HB3	6:C:507:HOH:O	2.18	0.43
1:F:33:ARG:HA	6:F:516:HOH:O	2.18	0.43
1:D:272:GLN:O	1:D:280:GLN:HG2	2.19	0.42
1:A:26:GLN:CD	1:E:239:GLN:OE1	2.62	0.42
1:E:10:GLY:HA2	1:E:13:LEU:HD13	2.01	0.42
1:C:302:LYS:HB2	4:C:401:PGE:H4	2.02	0.42
1:E:276:ASN:HB3	1:E:279:ILE:HD12	2.01	0.42
1:A:28:LEU:C	1:A:28:LEU:HD23	2.44	0.42
1:F:288:GLU:O	1:F:292:SER:HB3	2.20	0.42
1:B:239:GLN:OE1	1:C:26:GLN:OE1	2.38	0.42
1:D:16:MET:CE	1:D:35:LEU:HG	2.50	0.42
1:E:154:LEU:CD2	1:E:158:LEU:HD12	2.50	0.42
1:B:28:LEU:C	1:B:28:LEU:HD23	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:276:ASN:HB3	1:D:279:ILE:HD12	2.02	0.41
1:B:24:ASP:OD2	1:C:276:ASN:ND2	2.53	0.41
1:D:265:LEU:HD13	1:D:290:LEU:HD13	2.03	0.41
1:E:129:GLN:HE22	5:E:403:PG4:H31	1.86	0.41
1:A:227:VAL:HG13	1:A:267[B]:LYS:HD2	2.02	0.41
1:E:154:LEU:HD23	1:E:154:LEU:O	2.21	0.41
1:C:28:LEU:C	1:C:28:LEU:HD23	2.45	0.40
1:C:190:SER:N	6:C:510:HOH:O	2.53	0.40
1:E:291:GLN:NE2	6:E:519:HOH:O	2.54	0.40
1:F:272:GLN:O	1:F:280:GLN:HG2	2.21	0.40
1:F:154:LEU:HD23	1:F:154:LEU:O	2.21	0.40

All (8) 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)
6:E:648:HOH:O	6:F:629:HOH:O[2_656]	1.85	0.35
6:A:651:HOH:O	6:D:674:HOH:O[1_465]	1.92	0.28
6:E:682:HOH:O	6:F:659:HOH:O[2_656]	1.95	0.25
6:D:644:HOH:O	6:F:554:HOH:O[2_646]	2.01	0.19
6:E:677:HOH:O	6:F:597:HOH:O[2_656]	2.01	0.19
6:D:599:HOH:O	6:F:559:HOH:O[2_646]	2.05	0.15
1:D:26:GLN:NE2	1:F:239:GLN:OE1[2_646]	2.15	0.05
6:D:641:HOH:O	6:F:529:HOH:O[2_746]	2.17	0.03

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	303/302 (100%)	303 (100%)	0	0	100	100
1	B	301/302 (100%)	301 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	299/302 (99%)	296 (99%)	1 (0%)	2 (1%)	18	14
1	D	302/302 (100%)	302 (100%)	0	0	100	100
1	E	304/302 (101%)	304 (100%)	0	0	100	100
1	F	303/302 (100%)	301 (99%)	2 (1%)	0	100	100
All	All	1812/1812 (100%)	1807 (100%)	3 (0%)	2 (0%)	48	46

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	274	HIS
1	C	275	GLU

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	235/231 (102%)	226 (96%)	9 (4%)	29	29
1	B	234/231 (101%)	230 (98%)	4 (2%)	53	60
1	C	231/231 (100%)	224 (97%)	7 (3%)	36	38
1	D	235/231 (102%)	231 (98%)	4 (2%)	53	60
1	E	236/231 (102%)	231 (98%)	5 (2%)	47	52
1	F	233/231 (101%)	229 (98%)	4 (2%)	53	60
All	All	1404/1386 (101%)	1371 (98%)	33 (2%)	47	47

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	GLU
1	A	32	LEU
1	A	60	GLN
1	A	152	GLN
1	A	282[A]	GLU

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Mol	Chain	Res	Type
1	A	282[B]	GLU
1	A	291	GLN
1	A	292	SER
1	A	293	HIS
1	B	128	GLU
1	B	152	GLN
1	B	282	GLU
1	B	292	SER
1	C	37	GLN
1	C	266	GLU
1	C	267	LYS
1	C	280	GLN
1	C	292	SER
1	C	303[A]	ARG
1	C	303[B]	ARG
1	D	12	GLU
1	D	265	LEU
1	D	267	LYS
1	D	292	SER
1	E	29	GLN
1	E	33[A]	ARG
1	E	33[B]	ARG
1	E	242	LEU
1	E	292	SER
1	F	15	GLN
1	F	292	SER
1	F	298[A]	SER
1	F	298[B]	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	26	GLN
1	A	29	GLN
1	A	68	GLN
1	A	110	GLN
1	A	239	GLN
1	A	284	GLN
1	B	239	GLN
1	B	280	GLN
1	C	68	GLN
1	C	129	GLN

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Mol	Chain	Res	Type
1	C	236	GLN
1	C	239	GLN
1	C	274	HIS
1	C	280	GLN
1	C	284	GLN
1	D	37	GLN
1	D	236	GLN
1	E	37	GLN
1	E	68	GLN
1	E	85	ASN
1	E	152	GLN
1	E	197	GLN
1	E	211	ASN
1	F	270	GLN
1	F	291	GLN
1	F	293	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 37 ligands modelled in this entry, 18 are monoatomic - leaving 19 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
3	EDO	E	402	-	3,3,3	0.60	0	2,2,2	0.24	0
4	PGE	D	407	-	9,9,9	0.58	0	8,8,8	0.48	0
3	EDO	A	405	-	3,3,3	0.58	0	2,2,2	0.40	0
3	EDO	B	409	-	3,3,3	0.51	0	2,2,2	0.38	0
3	EDO	D	404	-	3,3,3	0.60	0	2,2,2	0.44	0
3	EDO	F	404	-	3,3,3	0.50	0	2,2,2	0.20	0
3	EDO	B	406	-	3,3,3	0.38	0	2,2,2	0.88	0
3	EDO	A	407	-	3,3,3	0.39	0	2,2,2	0.49	0
3	EDO	B	407	-	3,3,3	0.57	0	2,2,2	0.40	0
4	PGE	C	401	-	9,9,9	0.59	0	8,8,8	0.94	1 (12%)
3	EDO	A	408	-	3,3,3	0.58	0	2,2,2	0.24	0
5	PG4	E	404	-	12,12,12	0.70	0	11,11,11	0.46	0
3	EDO	B	408	-	3,3,3	0.46	0	2,2,2	0.44	0
3	EDO	A	406	-	3,3,3	0.48	0	2,2,2	0.29	0
3	EDO	D	405	-	3,3,3	0.53	0	2,2,2	0.18	0
4	PGE	E	405	-	9,9,9	0.67	0	8,8,8	1.32	1 (12%)
3	EDO	E	401	-	3,3,3	0.35	0	2,2,2	0.51	0
5	PG4	E	403	-	12,12,12	0.60	0	11,11,11	0.50	0
5	PG4	D	406	-	12,12,12	0.58	0	11,11,11	0.64	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	EDO	E	402	-	-	1/1/1/1	-
4	PGE	D	407	-	-	5/7/7/7	-
3	EDO	A	405	-	-	1/1/1/1	-
3	EDO	B	409	-	-	0/1/1/1	-
3	EDO	D	404	-	-	1/1/1/1	-
3	EDO	F	404	-	-	1/1/1/1	-
3	EDO	B	406	-	-	1/1/1/1	-
3	EDO	A	407	-	-	1/1/1/1	-
3	EDO	B	407	-	-	0/1/1/1	-
4	PGE	C	401	-	-	3/7/7/7	-
3	EDO	A	408	-	-	1/1/1/1	-
5	PG4	E	404	-	-	7/10/10/10	-
3	EDO	B	408	-	-	0/1/1/1	-
3	EDO	A	406	-	-	1/1/1/1	-
3	EDO	D	405	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PGE	E	405	-	-	5/7/7/7	-
3	EDO	E	401	-	-	1/1/1/1	-
5	PG4	E	403	-	-	9/10/10/10	-
5	PG4	D	406	-	-	5/10/10/10	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	405	PGE	O2-C2-C1	2.99	123.30	110.11
4	C	401	PGE	O3-C5-C6	2.19	119.77	110.11

There are no chirality outliers.

All (44) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	E	405	PGE	O2-C3-C4-O3
5	D	406	PG4	O4-C7-C8-O5
5	E	404	PG4	O2-C3-C4-O3
4	C	401	PGE	O1-C1-C2-O2
4	C	401	PGE	O3-C5-C6-O4
5	E	403	PG4	O1-C1-C2-O2
5	E	404	PG4	O4-C7-C8-O5
5	E	404	PG4	O1-C1-C2-O2
4	D	407	PGE	O1-C1-C2-O2
3	A	408	EDO	O1-C1-C2-O2
3	B	406	EDO	O1-C1-C2-O2
3	F	404	EDO	O1-C1-C2-O2
5	E	404	PG4	O3-C5-C6-O4
5	D	406	PG4	C8-C7-O4-C6
3	A	405	EDO	O1-C1-C2-O2
3	A	406	EDO	O1-C1-C2-O2
3	D	404	EDO	O1-C1-C2-O2
3	E	401	EDO	O1-C1-C2-O2
4	C	401	PGE	C6-C5-O3-C4
5	E	403	PG4	O2-C3-C4-O3
5	E	403	PG4	C3-C4-O3-C5
4	D	407	PGE	C6-C5-O3-C4
5	E	404	PG4	C8-C7-O4-C6
5	E	403	PG4	C1-C2-O2-C3

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Mol	Chain	Res	Type	Atoms
4	D	407	PGE	O2-C3-C4-O3
4	D	407	PGE	C4-C3-O2-C2
5	D	406	PG4	C1-C2-O2-C3
5	E	403	PG4	O4-C7-C8-O5
4	E	405	PGE	O3-C5-C6-O4
5	E	403	PG4	O3-C5-C6-O4
3	E	402	EDO	O1-C1-C2-O2
5	E	404	PG4	C1-C2-O2-C3
5	E	403	PG4	C4-C3-O2-C2
5	E	404	PG4	C6-C5-O3-C4
3	D	405	EDO	O1-C1-C2-O2
4	D	407	PGE	C1-C2-O2-C3
5	E	403	PG4	C5-C6-O4-C7
4	E	405	PGE	O1-C1-C2-O2
3	A	407	EDO	O1-C1-C2-O2
5	D	406	PG4	O1-C1-C2-O2
5	D	406	PG4	C3-C4-O3-C5
4	E	405	PGE	C4-C3-O2-C2
4	E	405	PGE	C6-C5-O3-C4
5	E	403	PG4	C8-C7-O4-C6

There are no ring outliers.

6 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	404	EDO	1	0
4	C	401	PGE	1	0
3	A	406	EDO	1	0
4	E	405	PGE	5	0
5	E	403	PG4	2	0
5	D	406	PG4	4	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	300/302 (99%)	-0.20	6 (2%) 65 64	9, 25, 49, 87	4 (1%)
1	B	299/302 (99%)	-0.22	1 (0%) 90 89	10, 27, 47, 78	3 (1%)
1	C	300/302 (99%)	0.37	17 (5%) 29 28	19, 38, 78, 103	1 (0%)
1	D	298/302 (98%)	-0.17	2 (0%) 84 84	10, 26, 54, 74	5 (1%)
1	E	301/302 (99%)	-0.05	3 (0%) 79 79	12, 29, 52, 83	5 (1%)
1	F	298/302 (98%)	0.10	13 (4%) 39 38	10, 28, 63, 91	7 (2%)
All	All	1796/1812 (99%)	-0.03	42 (2%) 61 60	9, 28, 59, 103	25 (1%)

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	297[A]	GLY	8.9
1	F	298[A]	SER	6.1
1	F	296[A]	GLY	5.1
1	C	309	TRP	5.0
1	C	10	GLY	4.4
1	F	295	SER	4.0
1	A	267[A]	LYS	3.9
1	C	279	ILE	3.7
1	F	294	GLY	3.7
1	A	309	TRP	3.7
1	C	274	HIS	3.7
1	E	309	TRP	3.6
1	E	9	PRO	3.5
1	D	170[A]	GLU	3.3
1	A	10	GLY	3.1
1	C	11	SER	3.1
1	B	293	HIS	3.1
1	C	280	GLN	3.0
1	A	293	HIS	3.0

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Mol	Chain	Res	Type	RSRZ
1	C	298	SER	2.8
1	F	273	SER	2.7
1	F	281	LYS	2.7
1	F	309	TRP	2.7
1	A	294	GLY	2.5
1	C	41	GLY	2.5
1	C	276	ASN	2.5
1	E	308	THR	2.4
1	C	273	SER	2.4
1	C	14	PRO	2.4
1	F	292	SER	2.3
1	F	293	HIS	2.3
1	C	287	LEU	2.3
1	F	291	GLN	2.2
1	C	283	ALA	2.1
1	C	277	GLU	2.1
1	C	282	GLU	2.1
1	A	297	GLY	2.1
1	F	23	PRO	2.1
1	F	290	LEU	2.0
1	D	19	GLN	2.0
1	C	281	LYS	2.0
1	C	290	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	EDO	D	405	4/4	0.66	0.23	78,82,85,87	0
3	EDO	B	407	4/4	0.67	0.19	56,66,72,77	0
4	PGE	D	407	10/10	0.67	0.24	77,84,88,90	0
3	EDO	A	405	4/4	0.69	0.25	60,66,73,78	0
4	PGE	E	405	10/10	0.71	0.23	64,80,88,89	0
3	EDO	E	401	4/4	0.74	0.14	63,64,65,67	0
5	PG4	E	404	13/13	0.75	0.21	39,75,89,90	0
3	EDO	F	404	4/4	0.76	0.20	57,65,67,69	0
3	EDO	E	402	4/4	0.79	0.17	57,63,68,72	0
5	PG4	D	406	13/13	0.80	0.16	56,68,77,77	0
5	PG4	E	403	13/13	0.81	0.18	62,70,76,78	0
4	PGE	C	401	10/10	0.83	0.13	52,59,67,69	0
3	EDO	A	408	4/4	0.83	0.17	55,57,58,61	0
3	EDO	B	408	4/4	0.84	0.17	57,57,59,65	0
3	EDO	A	407	4/4	0.85	0.16	55,56,58,65	0
3	EDO	D	404	4/4	0.88	0.16	57,65,68,68	0
3	EDO	A	406	4/4	0.89	0.12	50,53,54,59	0
3	EDO	B	406	4/4	0.90	0.13	46,46,48,58	0
3	EDO	B	409	4/4	0.92	0.14	46,47,49,53	0
2	CA	F	403	1/1	0.96	0.04	50,50,50,50	0
2	CA	D	402	1/1	0.97	0.05	22,22,22,22	0
2	CA	F	402	1/1	0.97	0.07	48,48,48,48	0
2	CA	A	404	1/1	0.98	0.06	35,35,35,35	0
2	CA	A	409	1/1	0.98	0.03	23,23,23,23	0
2	CA	B	401	1/1	0.98	0.04	25,25,25,25	0
2	CA	B	410	1/1	0.98	0.05	50,50,50,50	0
2	CA	D	401	1/1	0.98	0.07	41,41,41,41	0
2	CA	A	402	1/1	0.98	0.06	25,25,25,25	0
2	CA	D	403	1/1	0.98	0.06	28,28,28,28	0
2	CA	A	401	1/1	0.99	0.04	25,25,25,25	0
2	CA	B	402	1/1	0.99	0.03	25,25,25,25	0
2	CA	F	401	1/1	0.99	0.04	24,24,24,24	0
2	CA	B	403	1/1	0.99	0.05	30,30,30,30	0
2	CA	B	404	1/1	0.99	0.05	36,36,36,36	0
2	CA	B	405	1/1	0.99	0.06	36,36,36,36	0
2	CA	A	403	1/1	0.99	0.03	28,28,28,28	0
2	CA	A	410	1/1	0.99	0.03	28,28,28,28	0

6.5 Other polymers [i](#)

There are no such residues in this entry.