



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 11:59 AM UTC

PDB ID : 5B3G / pdb_00005b3g
Title : The crystal structure of the heterodimer of SHORT-ROOT and SCARECROW GRAS domains
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Deposited on : 2016-02-29
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

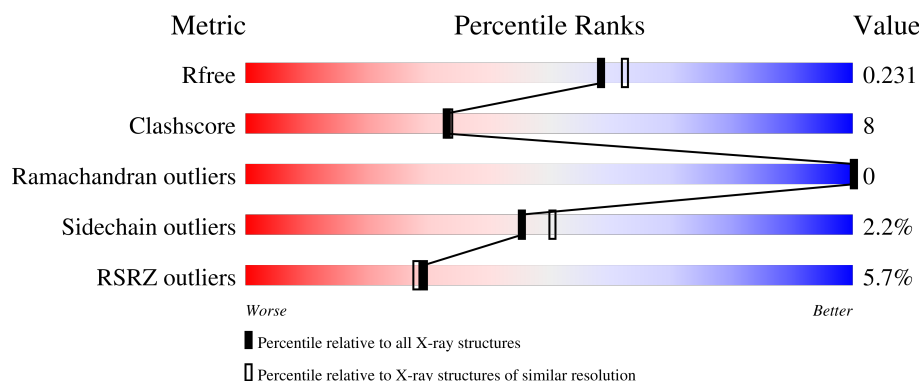
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

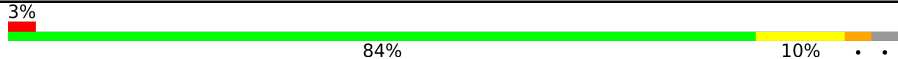
The reported resolution of this entry is 2.00 Å.

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	382	
2	B	475	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	PEG	A	704	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 6411 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 Protein SCARECROW.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	371	Total	C	N	O	S	0	1	0
			2885	1834	496	543	12			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	272	GLY	-	expression tag	UNP Q9M384
A	273	PRO	-	expression tag	UNP Q9M384

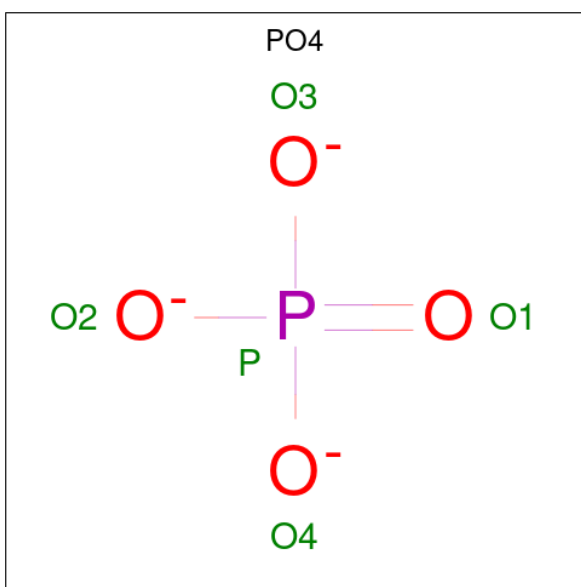
- Molecule 2 is a protein called Protein SHORT-ROOT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	406	Total	C	N	O	S	0	2	0
			3202	2014	568	599	21			

There are 3 discrepancies between the modelled and reference sequences:

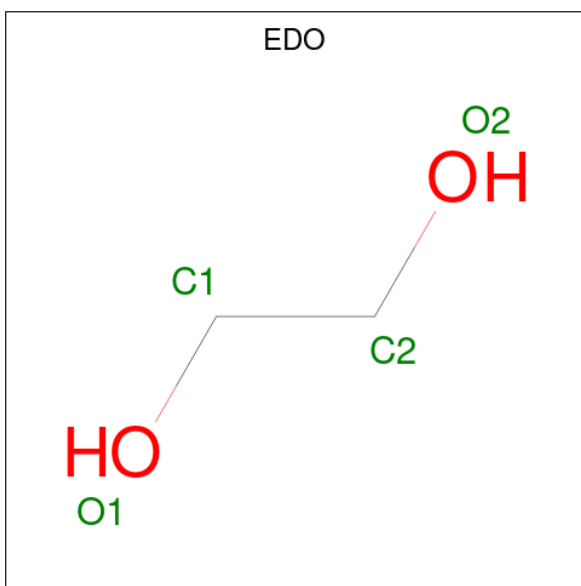
Chain	Residue	Modelled	Actual	Comment	Reference
B	57	GLY	-	expression tag	UNP Q9SZF7
B	58	PRO	-	expression tag	UNP Q9SZF7
B	233	SER	PRO	see sequence details	UNP Q9SZF7

- Molecule 3 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



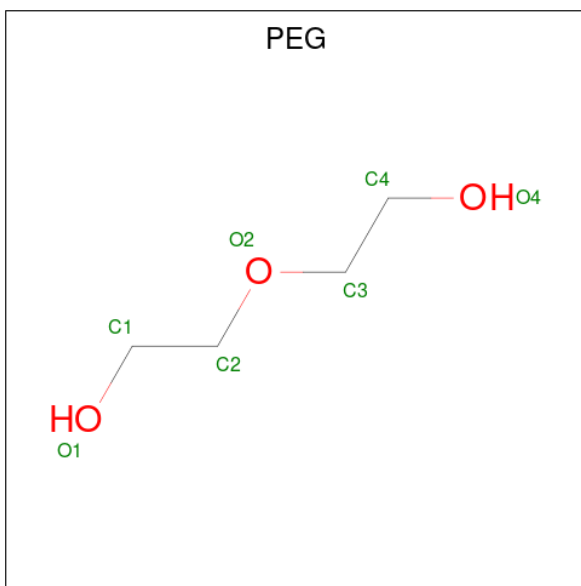
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	P	0	0
			5	4	1		

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



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

- Molecule 5 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



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

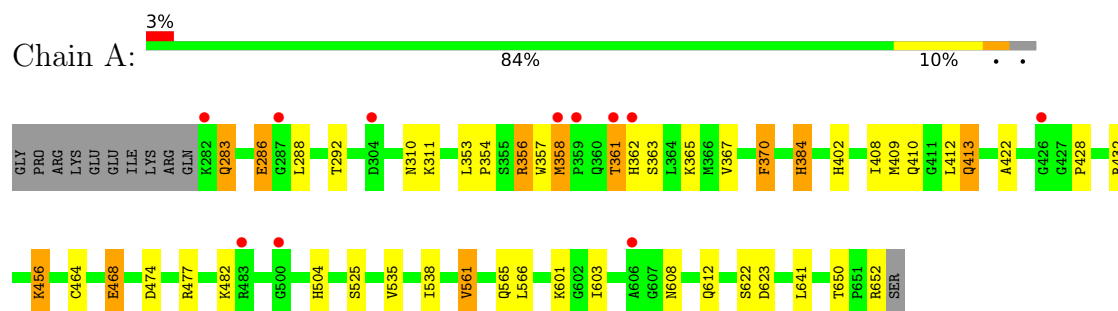
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	134	Total	O	0	0
			134	134		
6	B	152	Total	O	0	0
			152	152		

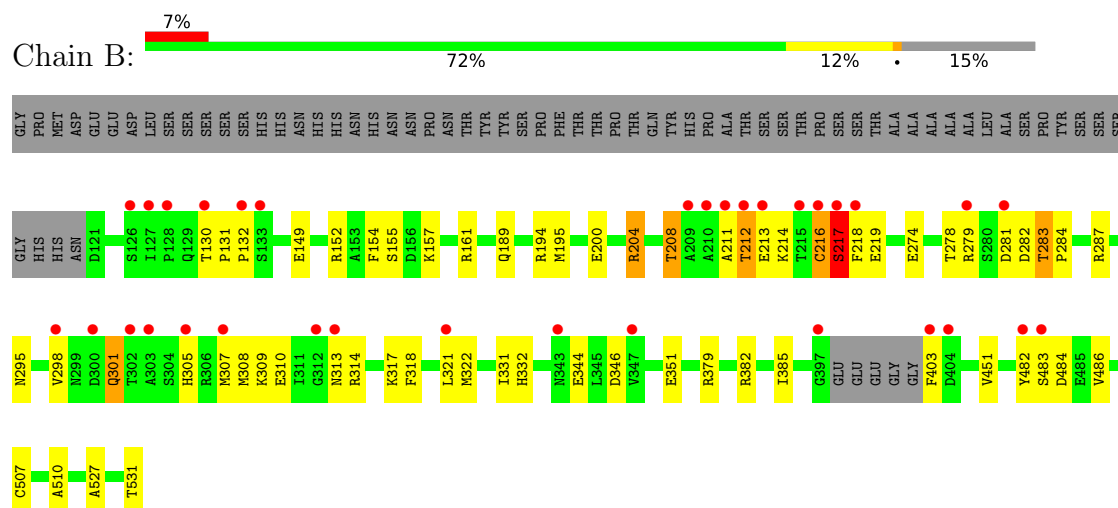
3 Residue-property plots [i](#)

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: Protein SCARECROW



• Molecule 2: Protein SHORT-ROOT



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	56.70Å 84.43Å 89.80Å 90.00° 92.66° 90.00°	Depositor
Resolution (Å)	33.10 – 2.00 33.10 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.3 (33.10-2.00) 99.3 (33.10-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.34 (at 2.00Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.183 , 0.230 0.188 , 0.231	Depositor DCC
R_{free} test set	2875 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	29.1	Xtriage
Anisotropy	0.019	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 46.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.032 for h,-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	6411	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.25% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, EDO, PEG

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	0.54	3/2948 (0.1%)	0.77	8/3997 (0.2%)
2	B	0.59	3/3274 (0.1%)	0.84	7/4437 (0.2%)
All	All	0.57	6/6222 (0.1%)	0.80	15/8434 (0.2%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	382	ARG	C-O	-7.01	1.20	1.23
1	A	409	MET	C-O	-6.21	1.18	1.24
2	B	208	THR	C-O	-5.69	1.17	1.24
1	A	370	PHE	C-O	-5.50	1.17	1.24
1	A	384	HIS	C-O	-5.42	1.17	1.24
2	B	204	ARG	C-O	-5.20	1.18	1.24

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	283	THR	N-CA-C	9.34	121.69	109.83
2	B	217	SER	N-CA-C	-8.36	102.16	111.28
2	B	282	ASP	N-CA-C	-8.02	98.26	110.70
2	B	279	ARG	N-CA-C	-7.74	102.84	111.28
1	A	413	GLN	N-CA-C	5.97	118.58	111.71
2	B	484	ASP	N-CA-C	-5.77	105.13	111.82
1	A	363	SER	N-CA-C	5.74	117.33	111.14
1	A	283	GLN	CA-C-N	5.65	128.42	120.28
1	A	283	GLN	C-N-CA	5.65	128.42	120.28
2	B	216	CYS	N-CA-C	-5.48	106.63	113.15
1	A	408	ILE	N-CA-C	5.42	117.82	111.05
2	B	212	THR	N-CA-C	5.37	118.24	109.59
1	A	286	GLU	N-CA-C	-5.29	105.52	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	358	MET	CA-C-N	-5.20	114.42	119.78
1	A	358	MET	C-N-CA	-5.20	114.42	119.78

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2885	0	2858	45	0
2	B	3202	0	3097	50	0
3	A	5	0	0	0	0
4	A	8	0	12	1	0
4	B	4	0	6	1	0
5	A	14	0	20	17	0
5	B	7	0	10	2	0
6	A	134	0	0	2	0
6	B	152	0	0	2	0
All	All	6411	0	6003	95	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (95) 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)
2:B:149:GLU:OE1	2:B:161:ARG:NH2	1.57	1.34
1:A:410:GLN:HB2	5:A:704:PEG:H31	1.16	1.16
2:B:214:LYS:HD2	2:B:216:CYS:HB2	1.31	1.06
1:A:410:GLN:HB2	5:A:704:PEG:C3	1.94	0.98
2:B:161:ARG:NH1	6:B:701:HOH:O	2.04	0.90
2:B:214:LYS:CD	2:B:216:CYS:HB2	2.01	0.88
1:A:412:LEU:H	5:A:704:PEG:H22	1.39	0.88
2:B:301:GLN:O	2:B:305:HIS:CD2	2.28	0.87
1:A:410:GLN:HG3	5:A:704:PEG:H42	1.63	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:370:PHE:HE2	5:A:704:PEG:H12	1.49	0.77
2:B:301:GLN:OE1	2:B:305:HIS:NE2	2.18	0.76
2:B:308:MET:HE1	5:B:602:PEG:H31	1.66	0.76
1:A:358:MET:HE2	1:A:362:HIS:HD2	1.53	0.73
2:B:321:LEU:O	2:B:321:LEU:HD23	1.88	0.72
1:A:361:THR:O	1:A:365:LYS:HG2	1.90	0.71
1:A:354:PRO:HB2	1:A:356:ARG:HD3	1.73	0.70
2:B:194:ARG:NE	2:B:403:PHE:CE1	2.60	0.69
2:B:301:GLN:O	2:B:305:HIS:HD2	1.74	0.69
1:A:370:PHE:CE2	5:A:704:PEG:H12	2.30	0.66
2:B:157:LYS:NZ	6:B:702:HOH:O	2.28	0.66
2:B:314:ARG:HH12	4:B:601:EDO:H22	1.61	0.65
1:A:525:SER:O	6:A:801:HOH:O	2.14	0.65
1:A:358:MET:HE2	1:A:362:HIS:CD2	2.32	0.64
2:B:321:LEU:HD23	2:B:321:LEU:C	2.24	0.63
1:A:412:LEU:H	5:A:704:PEG:C2	2.09	0.61
2:B:483:SER:HB3	2:B:486:VAL:H	1.65	0.61
2:B:218:PHE:CD1	2:B:307:MET:HE2	2.36	0.60
2:B:208:THR:O	2:B:212:THR:HG23	2.02	0.59
1:A:622:SER:OG	1:A:623:ASP:N	2.36	0.59
2:B:308:MET:HE1	5:B:602:PEG:H22	1.85	0.59
1:A:412:LEU:HB2	5:A:704:PEG:H11	1.85	0.57
2:B:287:ARG:NH2	2:B:346:ASP:O	2.35	0.57
1:A:370:PHE:HA	1:A:566:LEU:HD11	1.87	0.57
1:A:357:TRP:CD1	1:A:357:TRP:N	2.73	0.56
2:B:149:GLU:OE2	2:B:152:ARG:NH1	2.39	0.56
1:A:603:ILE:HD11	1:A:650:THR:HB	1.87	0.55
2:B:281:ASP:C	2:B:283:THR:H	2.15	0.54
1:A:412:LEU:HD23	5:A:705:PEG:H11	1.89	0.53
1:A:410:GLN:HB2	5:A:704:PEG:C4	2.37	0.52
1:A:384:HIS:HE1	5:A:704:PEG:H11	1.75	0.52
2:B:331:ILE:HD13	2:B:344:GLU:HG2	1.91	0.52
1:A:601:LYS:HE3	1:A:652:ARG:HA	1.92	0.52
2:B:281:ASP:C	2:B:283:THR:N	2.66	0.51
2:B:379:ARG:NH2	2:B:531:THR:O	2.40	0.51
1:A:410:GLN:NE2	5:A:704:PEG:O4	2.44	0.50
2:B:305:HIS:HA	2:B:332:HIS:CE1	2.47	0.50
1:A:353:LEU:HD21	1:A:357:TRP:HB2	1.93	0.50
2:B:194:ARG:HD2	2:B:451:VAL:O	2.12	0.49
2:B:274:GLU:O	2:B:278:THR:HG23	2.12	0.49
1:A:410:GLN:CG	5:A:704:PEG:H42	2.40	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:307:MET:HE1	2:B:308:MET:HE2	1.93	0.49
1:A:422:ALA:HA	1:A:428:PRO:HB3	1.94	0.49
2:B:321:LEU:C	2:B:321:LEU:CD2	2.85	0.49
2:B:155:SER:HA	2:B:403:PHE:HB3	1.94	0.49
1:A:283:GLN:O	1:A:286:GLU:HB2	2.13	0.48
1:A:410:GLN:CB	5:A:704:PEG:H31	2.11	0.48
2:B:212:THR:HA	2:B:213:GLU:HA	1.67	0.47
1:A:353:LEU:HD22	1:A:358:MET:HG2	1.96	0.47
1:A:468:GLU:OE2	1:A:477:ARG:NH2	2.33	0.47
1:A:358:MET:CE	1:A:362:HIS:HD2	2.26	0.47
1:A:402:HIS:CD2	1:A:432:ARG:HG2	2.51	0.46
1:A:535:VAL:O	1:A:538:ILE:HG22	2.16	0.46
1:A:504:HIS:ND1	4:A:702:EDO:H11	2.31	0.46
1:A:412:LEU:CB	5:A:704:PEG:H22	2.46	0.46
2:B:214:LYS:O	2:B:217:SER:N	2.49	0.45
2:B:211:ALA:HB3	2:B:298:VAL:HG11	1.98	0.45
1:A:288:LEU:O	1:A:292:THR:HG23	2.16	0.45
2:B:214:LYS:C	2:B:216:CYS:N	2.73	0.45
2:B:310:GLU:OE2	2:B:314:ARG:NE	2.32	0.45
1:A:474:ASP:OD1	1:A:477:ARG:HG2	2.17	0.44
2:B:214:LYS:CD	2:B:216:CYS:CB	2.85	0.44
2:B:154:PHE:CZ	2:B:195:MET:HE3	2.53	0.44
1:A:384:HIS:CD2	1:A:413:GLN:HB2	2.52	0.43
1:A:412:LEU:HB2	5:A:704:PEG:H22	2.00	0.43
2:B:200:GLU:OE2	2:B:204:ARG:NH1	2.51	0.43
2:B:130:THR:HA	2:B:131:PRO:HD3	1.91	0.43
2:B:295:ASN:ND2	2:B:298:VAL:HG22	2.34	0.43
2:B:507[B]:CYS:SG	2:B:510:ALA:HB3	2.59	0.43
1:A:456:LYS:HB3	1:A:456:LYS:HE3	1.58	0.43
1:A:565:GLN:NE2	6:A:810:HOH:O	2.52	0.42
1:A:412:LEU:N	5:A:704:PEG:H22	2.21	0.42
2:B:482:TYR:CD1	2:B:486:VAL:HG11	2.55	0.42
1:A:432:ARG:HD2	1:A:464:CYS:SG	2.59	0.42
2:B:287:ARG:NH2	2:B:351:GLU:OE1	2.42	0.42
2:B:131:PRO:HA	2:B:132:PRO:HD2	1.90	0.42
2:B:214:LYS:C	2:B:216:CYS:H	2.28	0.42
2:B:216:CYS:HA	2:B:219:GLU:HB3	2.02	0.42
2:B:385:ILE:HD11	2:B:527:ALA:HB1	2.00	0.42
2:B:313:ASN:OD1	2:B:317:LYS:HE3	2.19	0.42
1:A:384:HIS:CG	1:A:413:GLN:HB2	2.55	0.41
2:B:322:MET:HE3	2:B:322:MET:HA	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:318:PHE:O	2:B:322:MET:HB2	2.21	0.41
1:A:608:ASN:O	1:A:612:GLN:HG2	2.20	0.41
1:A:561:VAL:O	1:A:565:GLN:HB2	2.21	0.40
2:B:283:THR:HA	2:B:284:PRO:HD3	1.85	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	370/382 (97%)	363 (98%)	7 (2%)	0	100	100
2	B	404/475 (85%)	393 (97%)	11 (3%)	0	100	100
All	All	774/857 (90%)	756 (98%)	18 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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	309/318 (97%)	299 (97%)	10 (3%)	34	35
2	B	339/401 (84%)	335 (99%)	4 (1%)	63	70
All	All	648/719 (90%)	634 (98%)	14 (2%)	45	50

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	310	ASN
1	A	311	LYS
1	A	356	ARG
1	A	361	THR
1	A	367	VAL
1	A	456	LYS
1	A	468	GLU
1	A	482	LYS
1	A	561	VAL
1	A	641	LEU
2	B	189	GLN
2	B	217	SER
2	B	301	GLN
2	B	309	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	318	GLN
1	A	360	GLN
1	A	362	HIS
1	A	392	GLN
1	A	410	GLN
1	A	419	HIS
1	A	539	HIS
1	A	564	GLN
1	A	565	GLN
1	A	597	GLN
1	A	608	ASN
1	A	631	ASN
2	B	139	ASN
2	B	193	ASN
2	B	329	ASN
2	B	434	ASN
2	B	506	GLN

5.3.3 RNA ⓘ

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](#)

7 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	$\# Z > 2$
5	PEG	A	705	-	6,6,6	0.44	0	5,5,5	0.41	0
4	EDO	A	703	-	3,3,3	0.39	0	2,2,2	0.43	0
5	PEG	B	602	-	6,6,6	0.45	0	5,5,5	0.33	0
3	PO4	A	701	-	4,4,4	1.02	0	6,6,6	0.46	0
5	PEG	A	704	-	6,6,6	0.32	0	5,5,5	0.42	0
4	EDO	B	601	-	3,3,3	0.45	0	2,2,2	0.30	0
4	EDO	A	702	-	3,3,3	0.42	0	2,2,2	0.34	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
5	PEG	A	705	-	-	1/4/4/4	-
4	EDO	A	703	-	-	1/1/1/1	-
5	PEG	B	602	-	-	3/4/4/4	-
5	PEG	A	704	-	-	1/4/4/4	-
4	EDO	B	601	-	-	1/1/1/1	-
4	EDO	A	702	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	601	EDO	O1-C1-C2-O2
4	A	703	EDO	O1-C1-C2-O2
5	B	602	PEG	O1-C1-C2-O2
5	A	705	PEG	O2-C3-C4-O4
5	B	602	PEG	C4-C3-O2-C2
5	B	602	PEG	C1-C2-O2-C3
5	A	704	PEG	C1-C2-O2-C3

There are no ring outliers.

5 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	705	PEG	1	0
5	B	602	PEG	2	0
5	A	704	PEG	16	0
4	B	601	EDO	1	0
4	A	702	EDO	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	371/382 (97%)	0.03	11 (2%) 52 51	14, 31, 57, 84	1 (0%)
2	B	406/475 (85%)	0.36	33 (8%) 18 17	13, 34, 71, 99	2 (0%)
All	All	777/857 (90%)	0.20	44 (5%) 29 28	13, 32, 67, 99	3 (0%)

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	397	GLY	5.6
1	A	361	THR	5.2
2	B	298	VAL	3.8
2	B	217	SER	3.7
2	B	403	PHE	3.6
2	B	215	THR	3.6
2	B	212	THR	3.5
2	B	300	ASP	3.4
2	B	281	ASP	3.3
1	A	358	MET	3.3
2	B	303	ALA	3.3
2	B	213	GLU	2.8
2	B	343	ASN	2.8
2	B	211	ALA	2.8
1	A	606	ALA	2.8
2	B	307	MET	2.7
2	B	132	PRO	2.7
2	B	347	VAL	2.7
1	A	426	GLY	2.7
2	B	216	CYS	2.6
2	B	313	ASN	2.6
2	B	127	ILE	2.6
1	A	304	ASP	2.5
2	B	130	THR	2.5

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Mol	Chain	Res	Type	RSRZ
2	B	321	LEU	2.5
1	A	287	GLY	2.5
2	B	218	PHE	2.5
2	B	482	TYR	2.4
1	A	359	PRO	2.4
2	B	210	ALA	2.4
2	B	305	HIS	2.4
1	A	282	LYS	2.4
2	B	133	SER	2.3
1	A	500	GLY	2.3
2	B	279	ARG	2.3
2	B	128	PRO	2.3
2	B	404	ASP	2.3
1	A	362	HIS	2.2
2	B	126	SER	2.2
1	A	483	ARG	2.1
2	B	302	THR	2.1
2	B	209	ALA	2.1
2	B	483	SER	2.1
2	B	312	GLY	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	PEG	A	705	7/7	0.85	0.12	41,44,52,56	0
5	PEG	A	704	7/7	0.88	0.12	36,42,50,52	0
4	EDO	B	601	4/4	0.88	0.13	45,49,51,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	PEG	B	602	7/7	0.89	0.11	37,40,47,59	0
4	EDO	A	703	4/4	0.90	0.11	36,38,46,54	0
4	EDO	A	702	4/4	0.91	0.10	34,43,45,49	0
3	PO4	A	701	5/5	0.97	0.06	23,25,25,29	0

6.5 Other polymers [i](#)

There are no such residues in this entry.