



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 11:26 AM UTC

PDB ID : 8IDX / pdb_00008idx
Title : Structure of p205 HIN
Authors : Li, Y.L.; Jin, T.C.
Deposited on : 2023-02-14
Resolution : 1.75 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

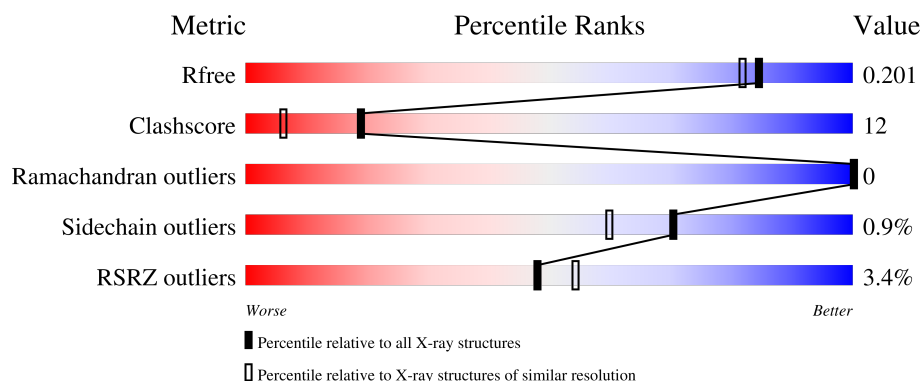
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.75 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	3183 (1.76-1.76)
Clashscore	190562	3299 (1.76-1.76)
Ramachandran outliers	187476	3274 (1.76-1.76)
Sidechain outliers	187428	3274 (1.76-1.76)
RSRZ outliers	180081	3183 (1.76-1.76)

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	221	3% 78% 9% 12%
1	B	221	3% 77% 10% 12%

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
2	PEG	A	502	-	-	X	-
2	PEG	A	503	-	-	X	-
2	PEG	B	502	-	-	X	-
2	PEG	B	503	-	-	X	-
3	EDO	A	511	-	-	X	-
4	PGE	B	501	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 3430 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 Interferon-activable protein 205-B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	194	Total	C	N	O	S	0	0	0
			1533	977	260	288	8			
1	B	194	Total	C	N	O	S	0	0	0
			1533	977	260	288	8			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	188	GLY	-	expression tag	UNP P0DOV1
A	189	SER	-	expression tag	UNP P0DOV1
A	190	VAL	-	expression tag	UNP P0DOV1
A	191	ASP	-	expression tag	UNP P0DOV1
A	405	ALA	-	expression tag	UNP P0DOV1
A	406	ALA	-	expression tag	UNP P0DOV1
A	407	ALA	-	expression tag	UNP P0DOV1
A	408	SER	-	expression tag	UNP P0DOV1
B	188	GLY	-	expression tag	UNP P0DOV1
B	189	SER	-	expression tag	UNP P0DOV1
B	190	VAL	-	expression tag	UNP P0DOV1
B	191	ASP	-	expression tag	UNP P0DOV1
B	405	ALA	-	expression tag	UNP P0DOV1
B	406	ALA	-	expression tag	UNP P0DOV1
B	407	ALA	-	expression tag	UNP P0DOV1
B	408	SER	-	expression tag	UNP P0DOV1

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



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

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



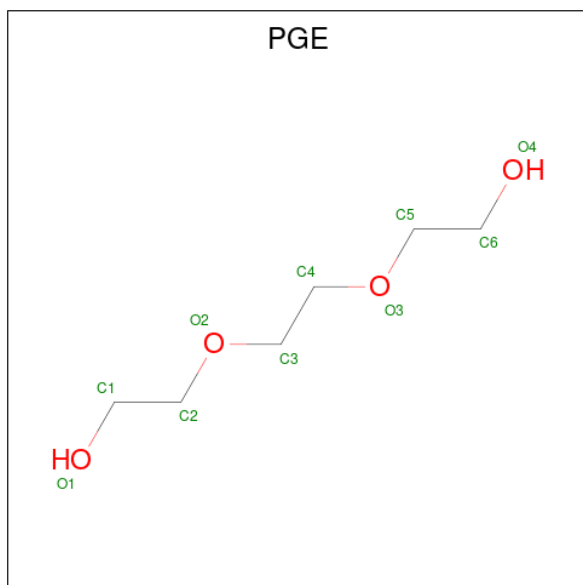
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0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

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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		

- Molecule 4 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: $C_6H_{14}O_4$).



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

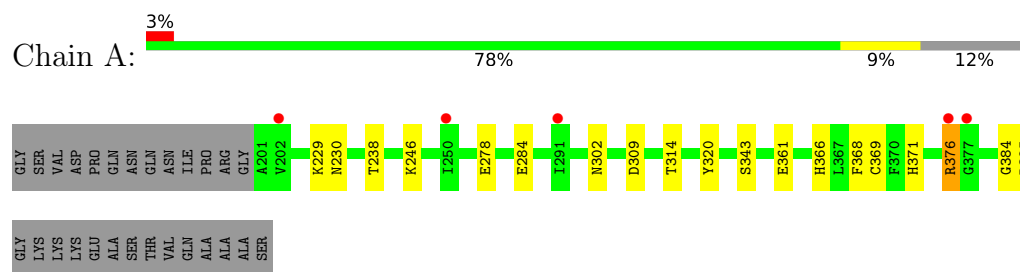
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	108	Total	O	0	0
			108	108		
5	B	101	Total	O	0	0
			101	101		

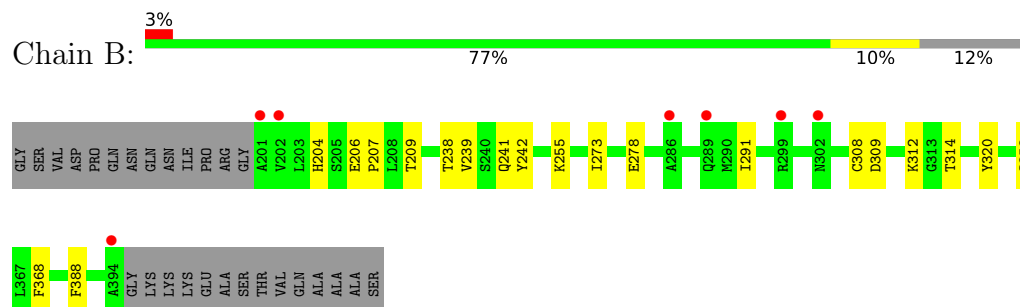
3 Residue-property plots [i](#)

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: Interferon-activable protein 205-B



- Molecule 1: Interferon-activable protein 205-B



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	48.64Å 51.12Å 56.58Å 103.15° 105.17° 108.29°	Depositor
Resolution (Å)	29.55 – 1.75 29.55 – 1.75	Depositor EDS
% Data completeness (in resolution range)	95.9 (29.55-1.75) 95.8 (29.55-1.75)	Depositor EDS
R_{merge}	0.02	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.90 (at 1.75Å)	Xtriage
Refinement program	PHENIX (1.15_3459: ???)	Depositor
R, R_{free}	0.172 , 0.199 0.177 , 0.201	Depositor DCC
R_{free} test set	2288 reflections (4.83%)	wwPDB-VP
Wilson B-factor (Å ²)	30.7	Xtriage
Anisotropy	0.370	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 48.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	3430	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.77% 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: PEG, PGE, 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	0.36	0/1567	0.57	0/2116
1	B	0.32	0/1567	0.52	0/2116
All	All	0.34	0/3134	0.55	0/4232

There are no bond length outliers.

There are no bond angle outliers.

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	1533	0	1527	33	0
1	B	1533	0	1527	33	0
2	A	21	0	30	16	0
2	B	14	0	20	13	0
3	A	60	0	90	12	0
3	B	40	0	60	9	0
4	B	20	0	28	14	0
5	A	108	0	0	4	0
5	B	101	0	0	5	0
All	All	3430	0	3282	77	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 12.

All (77) 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:A:385:ASP:N	2:A:503:PEG:H42	1.63	1.09
2:B:502:PEG:H41	2:B:502:PEG:H12	1.38	1.03
2:A:502:PEG:H12	5:A:687:HOH:O	1.75	0.86
1:A:386:HIS:H	2:A:503:PEG:C4	1.95	0.79
1:B:366:HIS:HB3	2:B:503:PEG:H21	1.64	0.79
1:A:385:ASP:H	2:A:503:PEG:H42	1.44	0.77
1:B:241:GLN:HB3	3:B:513:EDO:H11	1.67	0.77
1:B:209:THR:HG22	2:B:502:PEG:H42	1.65	0.77
2:B:502:PEG:H12	2:B:502:PEG:C4	2.00	0.77
1:A:376:ARG:HG3	1:A:376:ARG:HH11	1.49	0.76
4:B:501:PGE:H4	4:B:501:PGE:O4	1.84	0.76
1:B:368:PHE:CZ	2:B:503:PEG:H22	2.23	0.74
1:B:278:GLU:H	1:B:278:GLU:CD	1.97	0.73
1:A:229:LYS:HB3	3:A:511:EDO:H22	1.70	0.72
1:B:309:ASP:OD1	4:B:501:PGE:H6	1.91	0.70
1:A:371:HIS:CE1	2:A:503:PEG:H32	2.26	0.69
1:A:229:LYS:HB3	3:A:511:EDO:C2	2.23	0.69
2:A:502:PEG:O2	3:A:512:EDO:H22	1.92	0.69
1:A:229:LYS:HD3	3:A:511:EDO:H21	1.74	0.68
1:B:204:HIS:HB3	3:B:509:EDO:H22	1.75	0.68
1:B:364:LYS:NZ	5:B:602:HOH:O	2.26	0.67
1:A:384:GLY:C	2:A:503:PEG:H42	2.18	0.67
1:A:361:GLU:OE1	3:A:518:EDO:H22	1.95	0.66
1:A:376:ARG:HH11	1:A:376:ARG:CG	2.08	0.66
2:A:503:PEG:H11	3:A:506:EDO:O1	1.98	0.63
2:A:502:PEG:H42	5:A:691:HOH:O	1.99	0.62
1:B:238:THR:HA	2:B:502:PEG:H21	1.83	0.60
1:B:291:ILE:HB	2:B:502:PEG:H11	1.87	0.57
2:A:502:PEG:C1	5:A:687:HOH:O	2.41	0.57
1:B:238:THR:C	2:B:502:PEG:H21	2.30	0.56
1:B:309:ASP:OD2	4:B:501:PGE:H62	2.06	0.56
1:B:239:VAL:HG13	2:B:502:PEG:H22	1.87	0.55
1:A:366:HIS:HB2	1:A:390:LYS:HG2	1.88	0.55
1:B:239:VAL:N	2:B:502:PEG:H21	2.23	0.54
1:A:314:THR:HG22	1:B:314:THR:HG22	1.90	0.54
1:A:368:PHE:CZ	3:A:512:EDO:H11	2.43	0.54
1:B:309:ASP:OD1	4:B:501:PGE:C6	2.54	0.54
1:B:312:LYS:CE	4:B:501:PGE:H2	2.38	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:343:SER:C	3:B:513:EDO:H12	2.33	0.54
1:A:371:HIS:NE2	2:A:503:PEG:C3	2.73	0.52
1:B:309:ASP:OD2	4:B:501:PGE:C6	2.57	0.52
1:A:376:ARG:CG	1:A:376:ARG:NH1	2.73	0.52
1:B:238:THR:CA	2:B:502:PEG:H21	2.40	0.52
1:B:354:TRP:CZ3	3:B:510:EDO:H22	2.45	0.51
1:A:361:GLU:CG	3:A:518:EDO:H22	2.40	0.51
1:A:371:HIS:NE2	2:A:503:PEG:H32	2.26	0.51
1:A:386:HIS:H	2:A:503:PEG:H42	1.75	0.50
1:B:255:LYS:NZ	5:B:607:HOH:O	2.44	0.50
4:B:504:PGE:H5	5:B:688:HOH:O	2.11	0.50
1:A:230:ASN:H	3:A:511:EDO:H22	1.78	0.49
3:B:514:EDO:H11	5:B:673:HOH:O	2.13	0.48
2:A:501:PEG:H31	1:B:308:CYS:HB2	1.96	0.47
1:A:229:LYS:HB3	3:A:511:EDO:H21	1.95	0.46
1:A:284:GLU:H	1:A:284:GLU:CD	2.24	0.46
2:A:503:PEG:H11	2:A:503:PEG:H31	1.77	0.46
1:B:388:PHE:CZ	3:B:512:EDO:H11	2.50	0.46
1:A:376:ARG:NH1	1:A:376:ARG:HB2	2.31	0.46
1:A:246:LYS:NZ	1:A:369:CYS:SG	2.70	0.45
1:B:309:ASP:CG	4:B:501:PGE:C6	2.90	0.45
1:A:309:ASP:OD1	4:B:504:PGE:H12	2.16	0.45
1:A:238:THR:HA	3:A:515:EDO:H22	2.00	0.44
1:A:302:ASN:ND2	5:A:608:HOH:O	2.49	0.44
3:B:510:EDO:H21	3:B:512:EDO:O2	2.17	0.44
1:B:368:PHE:CE2	2:B:503:PEG:H32	2.53	0.43
1:B:242:TYR:CZ	3:B:506:EDO:H11	2.53	0.43
4:B:504:PGE:H1	4:B:504:PGE:H32	1.50	0.43
1:B:320:TYR:HB3	2:B:503:PEG:H31	1.99	0.43
1:A:320:TYR:H	4:B:501:PGE:H52	1.84	0.42
1:A:320:TYR:H	4:B:501:PGE:C5	2.32	0.42
1:B:309:ASP:CG	4:B:501:PGE:H6	2.44	0.42
1:A:386:HIS:H	2:A:503:PEG:H41	1.80	0.42
1:B:278:GLU:CD	1:B:278:GLU:N	2.73	0.42
1:B:273:ILE:HD11	4:B:504:PGE:H6	2.03	0.41
1:B:353:GLN:NE2	5:B:614:HOH:O	2.54	0.41
1:A:361:GLU:HG3	3:A:518:EDO:H22	2.03	0.41
1:A:314:THR:HG23	1:B:312:LYS:O	2.21	0.40
1:B:207:PRO:O	3:B:514:EDO:O2	2.28	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	192/221 (87%)	188 (98%)	4 (2%)	0	100	100
1	B	192/221 (87%)	188 (98%)	4 (2%)	0	100	100
All	All	384/442 (87%)	376 (98%)	8 (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	174/194 (90%)	172 (99%)	2 (1%)	65	52
1	B	174/194 (90%)	173 (99%)	1 (1%)	78	71
All	All	348/388 (90%)	345 (99%)	3 (1%)	70	60

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	278	GLU
1	A	376	ARG
1	B	206	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	230	ASN
1	A	295	ASN
1	B	259	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 ⓘ

32 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	EDO	A	506	-	3,3,3	0.45	0	2,2,2	0.45	0
3	EDO	A	511	-	3,3,3	0.54	0	2,2,2	0.22	0
3	EDO	A	518	-	3,3,3	0.52	0	2,2,2	0.44	0
3	EDO	A	517	-	3,3,3	0.44	0	2,2,2	0.34	0
3	EDO	A	509	-	3,3,3	0.44	0	2,2,2	0.39	0
3	EDO	A	515	-	3,3,3	0.45	0	2,2,2	0.27	0
3	EDO	B	506	-	3,3,3	0.42	0	2,2,2	0.32	0
4	PGE	B	504	-	9,9,9	0.53	0	8,8,8	0.21	0
2	PEG	A	502	-	6,6,6	0.53	0	5,5,5	0.34	0
3	EDO	B	509	-	3,3,3	0.57	0	2,2,2	0.48	0
3	EDO	A	513	-	3,3,3	0.44	0	2,2,2	0.42	0
3	EDO	A	508	-	3,3,3	0.44	0	2,2,2	0.42	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	PEG	B	502	-	6,6,6	0.61	0	5,5,5	0.17	0
2	PEG	A	503	-	6,6,6	0.63	0	5,5,5	0.21	0
3	EDO	A	505	-	3,3,3	0.45	0	2,2,2	0.39	0
3	EDO	A	516	-	3,3,3	0.42	0	2,2,2	0.34	0
3	EDO	B	505	-	3,3,3	0.44	0	2,2,2	0.40	0
4	PGE	B	501	-	9,9,9	0.67	0	8,8,8	0.40	0
3	EDO	B	513	-	3,3,3	0.45	0	2,2,2	0.36	0
3	EDO	A	510	-	3,3,3	0.44	0	2,2,2	0.24	0
3	EDO	A	507	-	3,3,3	0.44	0	2,2,2	0.34	0
3	EDO	B	507	-	3,3,3	0.44	0	2,2,2	0.43	0
3	EDO	B	512	-	3,3,3	0.42	0	2,2,2	0.44	0
3	EDO	A	514	-	3,3,3	0.44	0	2,2,2	0.34	0
2	PEG	A	501	-	6,6,6	0.50	0	5,5,5	0.24	0
2	PEG	B	503	-	6,6,6	0.64	0	5,5,5	0.43	0
3	EDO	B	511	-	3,3,3	0.44	0	2,2,2	0.43	0
3	EDO	B	510	-	3,3,3	0.44	0	2,2,2	0.22	0
3	EDO	A	512	-	3,3,3	0.60	0	2,2,2	0.44	0
3	EDO	B	514	-	3,3,3	0.42	0	2,2,2	0.39	0
3	EDO	A	504	-	3,3,3	0.41	0	2,2,2	0.37	0
3	EDO	B	508	-	3,3,3	0.48	0	2,2,2	0.53	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	A	506	-	-	1/1/1/1	-
3	EDO	A	511	-	-	0/1/1/1	-
3	EDO	A	518	-	-	1/1/1/1	-
3	EDO	A	517	-	-	0/1/1/1	-
3	EDO	A	509	-	-	1/1/1/1	-
3	EDO	A	515	-	-	0/1/1/1	-
3	EDO	B	506	-	-	0/1/1/1	-
4	PGE	B	504	-	-	5/7/7/7	-
2	PEG	A	502	-	-	2/4/4/4	-
3	EDO	B	509	-	-	1/1/1/1	-
3	EDO	A	513	-	-	0/1/1/1	-
3	EDO	A	508	-	-	0/1/1/1	-
2	PEG	B	502	-	-	3/4/4/4	-
2	PEG	A	503	-	-	3/4/4/4	-
3	EDO	A	505	-	-	0/1/1/1	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	A	516	-	-	0/1/1/1	-
3	EDO	B	505	-	-	0/1/1/1	-
4	PGE	B	501	-	-	3/7/7/7	-
3	EDO	B	513	-	-	0/1/1/1	-
3	EDO	A	510	-	-	0/1/1/1	-
3	EDO	A	507	-	-	1/1/1/1	-
3	EDO	B	507	-	-	0/1/1/1	-
3	EDO	B	512	-	-	0/1/1/1	-
3	EDO	A	514	-	-	0/1/1/1	-
2	PEG	A	501	-	-	1/4/4/4	-
2	PEG	B	503	-	-	3/4/4/4	-
3	EDO	B	511	-	-	0/1/1/1	-
3	EDO	B	510	-	-	0/1/1/1	-
3	EDO	A	512	-	-	0/1/1/1	-
3	EDO	B	514	-	-	1/1/1/1	-
3	EDO	A	504	-	-	0/1/1/1	-
3	EDO	B	508	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	501	PGE	C6-C5-O3-C4
4	B	504	PGE	C1-C2-O2-C3
2	A	503	PEG	C1-C2-O2-C3
4	B	504	PGE	O2-C3-C4-O3
2	B	502	PEG	O1-C1-C2-O2
2	B	502	PEG	C1-C2-O2-C3
2	A	502	PEG	O2-C3-C4-O4
2	B	503	PEG	O2-C3-C4-O4
4	B	501	PGE	O1-C1-C2-O2
2	A	503	PEG	O2-C3-C4-O4
4	B	504	PGE	O3-C5-C6-O4
3	B	514	EDO	O1-C1-C2-O2
4	B	504	PGE	C6-C5-O3-C4
4	B	501	PGE	C3-C4-O3-C5
2	A	502	PEG	C4-C3-O2-C2
2	B	502	PEG	O2-C3-C4-O4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	B	504	PGE	O1-C1-C2-O2
3	A	507	EDO	O1-C1-C2-O2
2	A	501	PEG	C1-C2-O2-C3
2	B	503	PEG	C1-C2-O2-C3
2	B	503	PEG	C4-C3-O2-C2
3	A	509	EDO	O1-C1-C2-O2
3	A	518	EDO	O1-C1-C2-O2
3	B	508	EDO	O1-C1-C2-O2
3	B	509	EDO	O1-C1-C2-O2
2	A	503	PEG	O1-C1-C2-O2
3	A	506	EDO	O1-C1-C2-O2

There are no ring outliers.

18 monomers are involved in 62 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	506	EDO	1	0
3	A	511	EDO	5	0
3	A	518	EDO	3	0
3	A	515	EDO	1	0
3	B	506	EDO	1	0
4	B	504	PGE	4	0
2	A	502	PEG	4	0
3	B	509	EDO	1	0
2	B	502	PEG	9	0
2	A	503	PEG	11	0
4	B	501	PGE	10	0
3	B	513	EDO	2	0
3	B	512	EDO	2	0
2	A	501	PEG	1	0
2	B	503	PEG	4	0
3	B	510	EDO	2	0
3	A	512	EDO	2	0
3	B	514	EDO	2	0

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	194/221 (87%)	0.33	6 (3%) 51 58	27, 39, 66, 100	0
1	B	194/221 (87%)	0.34	7 (3%) 46 52	28, 42, 71, 86	0
All	All	388/442 (87%)	0.34	13 (3%) 48 54	27, 41, 70, 100	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	394	ALA	3.7
1	B	394	ALA	3.3
1	B	201	ALA	3.1
1	B	286	ALA	3.0
1	B	202	VAL	2.8
1	A	291	ILE	2.7
1	A	377	GLY	2.5
1	A	376	ARG	2.3
1	B	289	GLN	2.3
1	B	299	ARG	2.3
1	B	302	ASN	2.2
1	A	250	ILE	2.1
1	A	202	VAL	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 ⓘ

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
2	PEG	A	502	7/7	0.71	0.20	66,77,82,84	0
3	EDO	A	505	4/4	0.76	0.14	64,72,74,77	0
3	EDO	A	507	4/4	0.81	0.14	57,69,71,76	0
3	EDO	A	510	4/4	0.81	0.25	74,77,80,81	0
2	PEG	A	503	7/7	0.82	0.20	40,63,67,71	0
2	PEG	A	501	7/7	0.82	0.18	55,61,66,68	0
3	EDO	A	509	4/4	0.85	0.13	69,71,77,79	0
3	EDO	B	509	4/4	0.85	0.13	50,60,71,76	0
3	EDO	B	511	4/4	0.85	0.17	73,78,79,80	0
3	EDO	A	516	4/4	0.86	0.16	55,64,67,67	0
3	EDO	A	511	4/4	0.86	0.15	47,48,49,59	0
3	EDO	A	514	4/4	0.86	0.14	52,57,58,58	0
3	EDO	B	513	4/4	0.86	0.14	48,55,58,71	0
3	EDO	A	517	4/4	0.87	0.14	67,70,76,82	0
3	EDO	B	514	4/4	0.87	0.13	67,70,77,79	0
4	PGE	B	504	10/10	0.87	0.15	46,54,61,64	0
3	EDO	A	518	4/4	0.88	0.11	54,59,60,64	0
3	EDO	B	507	4/4	0.88	0.15	67,68,70,74	0
3	EDO	A	506	4/4	0.88	0.15	77,79,84,85	0
3	EDO	B	510	4/4	0.88	0.14	51,51,52,61	0
3	EDO	B	512	4/4	0.89	0.12	53,54,61,74	0
3	EDO	B	506	4/4	0.89	0.15	66,66,68,72	0
3	EDO	A	515	4/4	0.89	0.13	52,55,55,60	0
4	PGE	B	501	10/10	0.89	0.14	47,64,70,78	0
3	EDO	B	508	4/4	0.89	0.14	51,51,58,66	0
3	EDO	B	505	4/4	0.90	0.15	68,71,75,75	0
2	PEG	B	503	7/7	0.90	0.11	47,54,58,69	0
3	EDO	A	508	4/4	0.91	0.11	59,62,62,75	0
3	EDO	A	512	4/4	0.92	0.13	61,64,67,69	0
3	EDO	A	504	4/4	0.93	0.11	47,50,50,52	0
2	PEG	B	502	7/7	0.93	0.11	57,60,70,70	0
3	EDO	A	513	4/4	0.95	0.07	44,48,50,50	0

6.5 Other polymers ⓘ

There are no such residues in this entry.