



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:21 PM UTC

PDB ID : 4HDM / pdb_00004hdm
Title : Crystal Structure of ArsAB in Complex with p-cresol
Authors : Newmister, S.A.; Chan, C.H.; Escalante-Semerena, J.C.; Rayment, I.
Deposited on : 2012-10-02
Resolution : 1.95 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

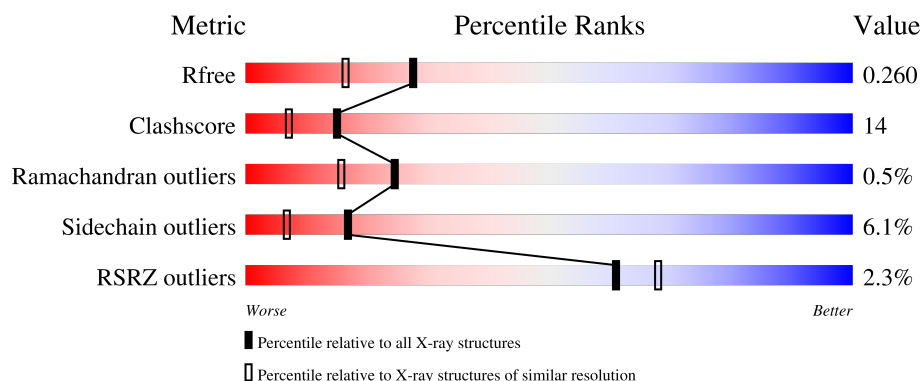
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

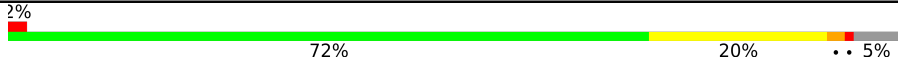
The reported resolution of this entry is 1.95 Å.

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	3494 (1.96-1.96)
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (1.96-1.96)

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	348	
2	B	350	

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 4990 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 ArsA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	331	2445	1539	427	459	20	0	4	0

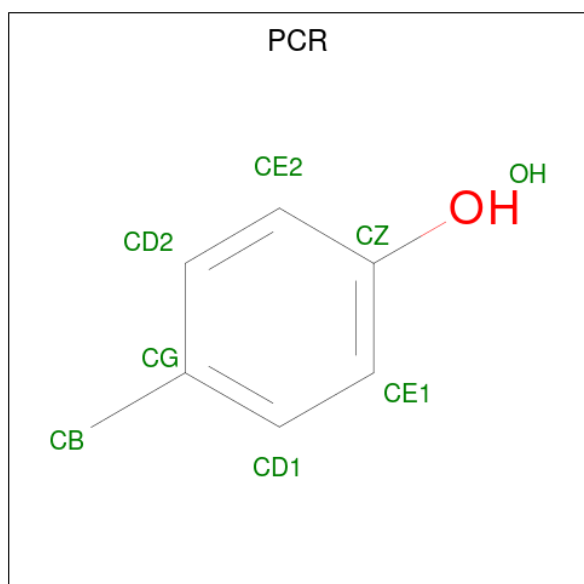
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP F6MZ55
A	0	GLY	-	expression tag	UNP F6MZ55

- Molecule 2 is a protein called ArsB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	326	2348	1476	419	433	20	0	2	0

- Molecule 3 is P-CRESOL (CCD ID: PCR) (formula: C₇H₈O).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			8	7	1		

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



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

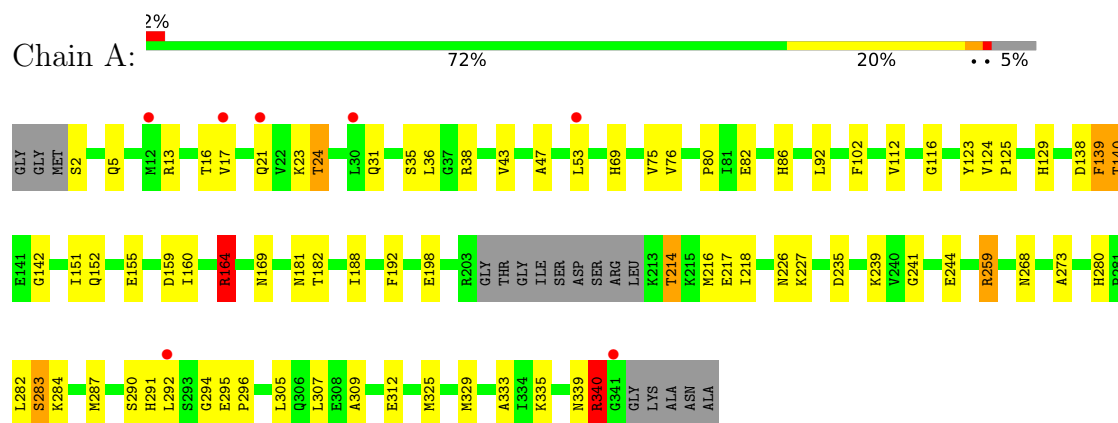
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	63	Total	O	0	0
			63	63		
5	B	122	Total	O	0	0
			122	122		

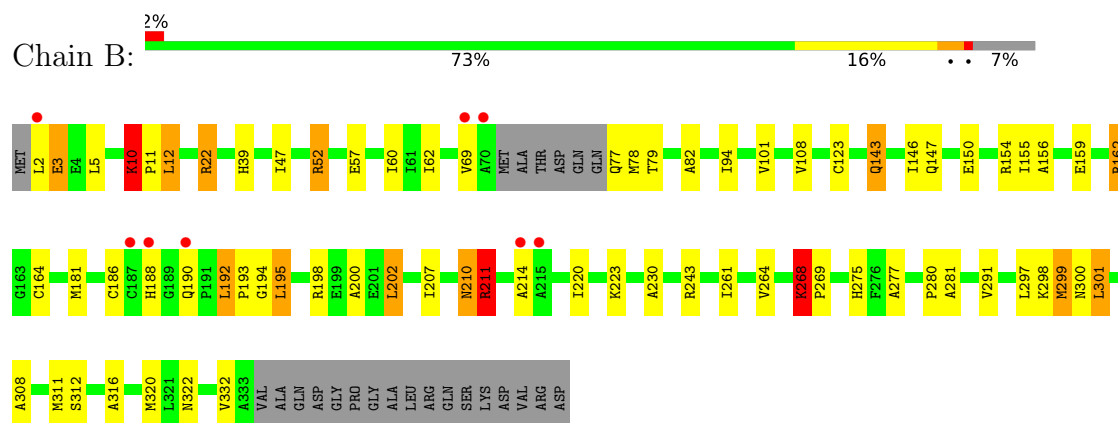
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: ArsaA



• Molecule 2: ArsB



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	52.56Å 77.94Å 152.18Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 1.95 50.00 – 1.95	Depositor EDS
% Data completeness (in resolution range)	99.3 (50.00-1.95) 99.3 (50.00-1.95)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.13 (at 1.95Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.195 , 0.256 0.197 , 0.260	Depositor DCC
R_{free} test set	2328 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	33.5	Xtriage
Anisotropy	0.026	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 33.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	4990	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.88% 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: PCR, 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	1.26	4/2490 (0.2%)	1.26	5/3372 (0.1%)
2	B	1.43	5/2384 (0.2%)	1.37	22/3237 (0.7%)
All	All	1.35	9/4874 (0.2%)	1.31	27/6609 (0.4%)

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	159	GLU	N-CA	5.92	1.53	1.46
2	B	268	LYS	C-O	-5.80	1.19	1.24
1	A	291	HIS	CA-C	-5.72	1.45	1.52
1	A	129	HIS	CE1-NE2	5.45	1.38	1.32
2	B	277	ALA	N-CA	5.24	1.52	1.45
2	B	5	LEU	C-O	-5.21	1.18	1.24
2	B	320	MET	C-O	5.21	1.30	1.24
1	A	47	ALA	C-O	-5.13	1.18	1.24
1	A	86	HIS	CG-CD2	5.10	1.41	1.35

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	52	ARG	NE-CZ-NH1	11.12	132.62	121.50
2	B	52	ARG	NE-CZ-NH2	-8.08	111.93	119.20
2	B	52	ARG	CB-CG-CD	7.97	129.63	111.30
2	B	52	ARG	CD-NE-CZ	6.62	133.67	124.40
2	B	268	LYS	CA-CB-CG	6.52	127.14	114.10
2	B	211	ARG	CA-C-N	-5.80	113.81	119.90
2	B	211	ARG	C-N-CA	-5.80	113.81	119.90
1	A	294	GLY	N-CA-C	-5.76	99.52	113.18
1	A	160	ILE	N-CA-C	-5.62	105.02	110.42
2	B	10	LYS	N-CA-C	5.62	117.76	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	322	ASN	N-CA-C	5.49	117.34	111.36
2	B	156	ALA	N-CA-C	-5.44	105.26	111.14
2	B	299	MET	CA-C-N	5.44	130.78	122.24
2	B	299	MET	C-N-CA	5.44	130.78	122.24
2	B	210	ASN	N-CA-C	5.44	119.97	113.23
2	B	291	VAL	CA-C-N	-5.41	115.01	120.31
2	B	291	VAL	C-N-CA	-5.41	115.01	120.31
1	A	291	HIS	CB-CA-C	-5.21	101.77	109.90
2	B	143	GLN	CA-C-N	5.18	127.17	120.44
2	B	143	GLN	C-N-CA	5.18	127.17	120.44
2	B	188	HIS	N-CA-C	5.10	116.53	111.07
2	B	192	LEU	CA-C-N	-5.08	114.51	119.99
2	B	192	LEU	C-N-CA	-5.08	114.51	119.99
2	B	230	ALA	CA-C-N	-5.07	113.79	120.22
2	B	230	ALA	C-N-CA	-5.07	113.79	120.22
1	A	192	PHE	N-CA-C	5.05	117.44	111.33
1	A	164	ARG	CD-NE-CZ	5.04	131.46	124.40

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	2445	0	2515	81	0
2	B	2348	0	2437	67	0
3	A	8	0	8	0	0
4	B	4	0	6	0	0
5	A	63	0	0	6	0
5	B	122	0	0	14	0
All	All	4990	0	4966	134	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 14.

All (134) 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:339:ASN:HA	1:A:340:ARG:CB	1.78	1.13
2:B:211:ARG:HG3	2:B:211:ARG:HH11	1.10	1.10
2:B:22:ARG:HG3	2:B:22:ARG:HH11	1.19	1.05
1:A:339:ASN:HA	1:A:340:ARG:HB2	1.02	1.02
1:A:36:LEU:HD22	2:B:299:MET:CE	1.89	1.01
1:A:339:ASN:CA	1:A:340:ARG:HB2	1.87	1.01
1:A:102:PHE:HE2	1:A:325[A]:MET:HE3	1.28	0.97
1:A:80:PRO:HB2	1:A:82:GLU:OE1	1.65	0.96
2:B:57:GLU:HG3	5:B:1114:HOH:O	1.65	0.95
1:A:295:GLU:HB2	1:A:296:PRO:HD2	1.52	0.92
1:A:102:PHE:HE2	1:A:325[A]:MET:CE	1.84	0.90
2:B:308:ALA:HA	2:B:311:MET:HE2	1.53	0.90
1:A:259:ARG:HG2	1:A:259:ARG:HH11	1.35	0.90
1:A:36:LEU:HD22	2:B:299:MET:HE2	1.53	0.90
2:B:211:ARG:HH11	2:B:211:ARG:CG	1.85	0.89
1:A:102:PHE:CE2	1:A:325[A]:MET:CE	2.55	0.89
2:B:181:MET:HE1	2:B:280:PRO:HB2	1.53	0.88
2:B:211:ARG:HG3	2:B:211:ARG:NH1	1.85	0.86
1:A:102:PHE:CE2	1:A:325[A]:MET:HE3	2.12	0.85
1:A:339:ASN:OD1	1:A:340:ARG:HB3	1.79	0.83
2:B:60:ILE:HD11	2:B:311:MET:HE1	1.59	0.83
2:B:143:GLN:O	2:B:147:GLN:HG3	1.78	0.82
1:A:287[A]:MET:HE3	1:A:307:LEU:HD11	1.60	0.81
2:B:243:ARG:HD3	5:B:1078:HOH:O	1.80	0.79
1:A:214:THR:HG23	5:A:954:HOH:O	1.83	0.78
2:B:146:ILE:O	2:B:150:GLU:HG3	1.84	0.77
2:B:22:ARG:HG3	2:B:22:ARG:NH1	1.95	0.76
1:A:312:GLU:OE2	5:A:918:HOH:O	2.03	0.76
1:A:164:ARG:NH1	1:A:169:ASN:OD1	2.17	0.76
1:A:164:ARG:HH11	1:A:164:ARG:HG3	1.51	0.75
1:A:280:HIS:O	1:A:283:SER:HB2	1.89	0.73
2:B:243:ARG:CD	5:B:1078:HOH:O	2.35	0.73
1:A:325[A]:MET:HE1	2:B:316:ALA:CB	2.19	0.71
1:A:36:LEU:CD2	2:B:299:MET:HE2	2.20	0.70
1:A:325[A]:MET:HE1	2:B:316:ALA:HB1	1.74	0.69
1:A:38:ARG:NH2	2:B:298:LYS:HE3	2.10	0.66
1:A:2:SER:OG	1:A:5:GLN:HG2	1.96	0.66
2:B:214:ALA:HA	2:B:220:ILE:HD11	1.79	0.64
1:A:69:HIS:HE1	1:A:244:GLU:OE2	1.79	0.64
2:B:308:ALA:HA	2:B:311:MET:CE	2.27	0.64
1:A:339:ASN:CA	1:A:340:ARG:CB	2.58	0.64
1:A:295:GLU:HB2	1:A:296:PRO:CD	2.27	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:164:ARG:NH1	1:A:164:ARG:HG3	2.11	0.62
2:B:39:HIS:HE1	5:B:1011:HOH:O	1.82	0.62
1:A:214:THR:CG2	1:A:216:MET:CG	2.78	0.62
1:A:102:PHE:CD2	1:A:325[A]:MET:HE2	2.35	0.62
1:A:36:LEU:HD22	2:B:299:MET:HE3	1.81	0.61
2:B:52:ARG:HD2	5:B:1002:HOH:O	2.00	0.61
1:A:214:THR:CG2	1:A:216:MET:HG2	2.31	0.61
1:A:284:LYS:HA	1:A:287[A]:MET:HE2	1.82	0.61
1:A:284:LYS:HB2	1:A:287[A]:MET:HE2	1.82	0.61
1:A:295:GLU:CB	1:A:296:PRO:HD2	2.29	0.60
2:B:195:LEU:HD12	2:B:195:LEU:H	1.67	0.60
1:A:284:LYS:CB	1:A:287[A]:MET:HE2	2.32	0.60
2:B:10:LYS:HB3	2:B:11:PRO:HD2	1.85	0.59
2:B:164:CYS:N	5:B:1115:HOH:O	2.33	0.59
1:A:214:THR:HB	1:A:217:GLU:OE1	2.03	0.59
1:A:214:THR:HG22	1:A:217:GLU:H	1.68	0.59
2:B:39:HIS:HD2	5:B:1042:HOH:O	1.86	0.58
1:A:102:PHE:CD2	1:A:325[A]:MET:CE	2.87	0.58
1:A:164:ARG:HG3	1:A:169:ASN:OD1	2.04	0.58
1:A:335:LYS:O	5:A:933:HOH:O	2.17	0.57
1:A:82:GLU:H	1:A:82:GLU:CD	2.13	0.57
1:A:216:MET:HG2	5:A:954:HOH:O	2.04	0.56
2:B:69:VAL:HG13	2:B:69:VAL:O	2.05	0.56
1:A:214:THR:CG2	1:A:216:MET:HG3	2.36	0.55
2:B:195:LEU:HD22	2:B:200:ALA:HA	1.87	0.55
2:B:2:LEU:HB3	2:B:3:GLU:OE2	2.06	0.55
1:A:214:THR:HG21	1:A:216:MET:CG	2.37	0.55
1:A:35:SER:H	2:B:300:ASN:HB2	1.72	0.55
2:B:101:VAL:HG21	2:B:311:MET:HE3	1.90	0.54
2:B:108:VAL:HG21	2:B:155:ILE:HD13	1.89	0.54
1:A:259:ARG:HG2	1:A:259:ARG:NH1	2.11	0.53
2:B:186[A]:CYS:SG	2:B:207:ILE:HG12	2.48	0.53
1:A:138:ASP:OD1	1:A:140:THR:HB	2.08	0.53
2:B:268:LYS:HD2	2:B:268:LYS:C	2.34	0.53
1:A:35:SER:H	2:B:300:ASN:CB	2.22	0.51
1:A:139:PHE:HA	1:A:142:GLY:O	2.10	0.51
1:A:226:ASN:HB3	1:A:239:LYS:HD3	1.93	0.51
1:A:102:PHE:HD2	1:A:325[A]:MET:HE2	1.73	0.51
1:A:214:THR:HG21	1:A:216:MET:HG3	1.92	0.51
2:B:211:ARG:CG	2:B:211:ARG:NH1	2.55	0.51
2:B:154:ARG:NH2	5:B:1116:HOH:O	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:332:VAL:O	2:B:332:VAL:CG1	2.59	0.50
2:B:60:ILE:HD11	2:B:311:MET:CE	2.36	0.50
1:A:69:HIS:CD2	5:A:908:HOH:O	2.64	0.50
2:B:195:LEU:HD13	2:B:195:LEU:O	2.11	0.49
1:A:43:VAL:HB	1:A:333:ALA:HB1	1.94	0.49
2:B:2:LEU:N	5:B:1088:HOH:O	2.45	0.49
1:A:287[A]:MET:HE1	1:A:305:LEU:HD22	1.96	0.48
2:B:268:LYS:HD2	2:B:268:LYS:O	2.13	0.48
1:A:31:GLN:HB3	2:B:78:MET:HE2	1.96	0.48
1:A:164:ARG:HH11	1:A:164:ARG:CG	2.23	0.47
1:A:36:LEU:CD2	2:B:299:MET:CE	2.77	0.47
2:B:62:ILE:HD11	2:B:94:ILE:HG12	1.96	0.47
2:B:198:ARG:O	2:B:202:LEU:HB2	2.15	0.47
2:B:162:ARG:NH2	5:B:1056:HOH:O	2.47	0.46
2:B:47:ILE:O	2:B:243:ARG:HD2	2.15	0.46
1:A:284:LYS:CA	1:A:287[A]:MET:HE2	2.45	0.46
1:A:69:HIS:CE1	1:A:181:ASN:HB3	2.51	0.46
1:A:290:SER:O	1:A:309:ALA:HB1	2.15	0.45
1:A:216:MET:HE3	1:A:216:MET:HB2	1.79	0.45
2:B:192:LEU:O	2:B:195:LEU:HD12	2.17	0.44
2:B:123[A]:CYS:SG	5:B:1117:HOH:O	2.62	0.44
2:B:280:PRO:O	2:B:281:ALA:HB3	2.17	0.44
2:B:332:VAL:O	2:B:332:VAL:HG12	2.17	0.44
1:A:155:GLU:O	1:A:159:ASP:HB2	2.18	0.44
2:B:12:LEU:HD22	2:B:269:PRO:HB3	1.99	0.44
1:A:273:ALA:HB1	1:A:287[A]:MET:SD	2.58	0.44
2:B:275:HIS:HD2	5:B:1025:HOH:O	2.01	0.43
1:A:235:ASP:OD1	1:A:239:LYS:NZ	2.51	0.43
1:A:92:LEU:HD11	1:A:112:VAL:HB	1.99	0.43
1:A:329:MET:HE2	2:B:297:LEU:HD11	2.00	0.43
2:B:211:ARG:HB3	5:B:1112:HOH:O	2.17	0.43
2:B:261:ILE:HG21	2:B:268:LYS:HB2	1.99	0.43
2:B:194:GLY:H	2:B:280:PRO:HB3	1.84	0.43
2:B:243:ARG:HD2	5:B:1078:HOH:O	2.11	0.43
1:A:123:TYR:O	1:A:125:PRO:HD3	2.19	0.42
2:B:210:ASN:HB3	2:B:223:LYS:HD3	2.02	0.42
1:A:75:VAL:HG12	1:A:218:ILE:HD13	2.02	0.42
1:A:124:VAL:HA	1:A:125:PRO:HD3	1.81	0.42
2:B:193:PRO:HA	2:B:194:GLY:HA2	1.61	0.42
1:A:151:ILE:O	1:A:155:GLU:HG3	2.20	0.41
1:A:182:THR:HA	1:A:268:ASN:HD21	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:152:GLN:HG3	5:A:960:HOH:O	2.19	0.41
2:B:79:THR:O	2:B:82:ALA:HB3	2.20	0.41
1:A:325[A]:MET:HE1	2:B:316:ALA:HB2	2.01	0.41
1:A:36:LEU:HD23	2:B:301:LEU:HB2	2.02	0.41
1:A:198:GLU:HG3	1:A:216:MET:SD	2.60	0.41
1:A:164:ARG:NH1	1:A:164:ARG:CG	2.83	0.41
1:A:21:GLN:O	1:A:24:THR:HG22	2.21	0.40
1:A:80:PRO:CB	1:A:82:GLU:OE1	2.52	0.40
1:A:188:ILE:HD11	1:A:241:GLY:HA2	2.02	0.40
2:B:311:MET:HE3	2:B:311:MET:HB2	1.45	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	331/348 (95%)	305 (92%)	24 (7%)	2 (1%)	21	12
2	B	324/350 (93%)	309 (95%)	14 (4%)	1 (0%)	36	28
All	All	655/698 (94%)	614 (94%)	38 (6%)	3 (0%)	24	16

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	340	ARG
2	B	190	GLN
1	A	116	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	258/264 (98%)	241 (93%)	17 (7%)	15	5
2	B	238/256 (93%)	225 (94%)	13 (6%)	19	8
All	All	496/520 (95%)	466 (94%)	30 (6%)	17	7

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	ARG
1	A	16	THR
1	A	17	VAL
1	A	23	LYS
1	A	24	THR
1	A	53	LEU
1	A	76	VAL
1	A	139	PHE
1	A	140	THR
1	A	164	ARG
1	A	214	THR
1	A	227	LYS
1	A	259	ARG
1	A	282	LEU
1	A	283	SER
1	A	292	LEU
1	A	340	ARG
2	B	3	GLU
2	B	10	LYS
2	B	12	LEU
2	B	22	ARG
2	B	77	GLN
2	B	162	ARG
2	B	195	LEU
2	B	202	LEU
2	B	211	ARG
2	B	264	VAL

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Mol	Chain	Res	Type
2	B	268	LYS
2	B	301	LEU
2	B	312	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	69	HIS
1	A	268	ASN
1	A	277	ASN
1	A	280	HIS
2	B	39	HIS
2	B	91	GLN
2	B	143	GLN
2	B	147	GLN
2	B	275	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](#)

2 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	PCR	A	801	-	8,8,8	0.81	0	10,10,10	1.24	2 (20%)
4	EDO	B	901	-	3,3,3	0.73	0	2,2,2	0.21	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	PCR	A	801	-	-	-	0/1/1/1
4	EDO	B	901	-	-	1/1/1/1	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	801	PCR	CD2-CE2-CZ	-2.47	117.27	119.88
3	A	801	PCR	CE2-CD2-CG	2.03	123.71	121.37

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	901	EDO	O1-C1-C2-O2

There are no ring outliers.

No monomer is involved in short contacts.

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	331/348 (95%)	0.40	7 (2%) 63 70	17, 42, 67, 103	4 (1%)
2	B	326/350 (93%)	-0.00	8 (2%) 58 65	20, 33, 71, 96	2 (0%)
All	All	657/698 (94%)	0.20	15 (2%) 61 68	17, 38, 69, 103	6 (0%)

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	2	LEU	3.5
2	B	69	VAL	3.3
1	A	341	GLY	3.3
1	A	21	GLN	3.0
2	B	70	ALA	2.9
1	A	30	LEU	2.9
2	B	187	CYS	2.5
1	A	292	LEU	2.5
2	B	214	ALA	2.3
2	B	215	ALA	2.3
1	A	53	LEU	2.2
2	B	190	GLN	2.2
2	B	188	HIS	2.1
1	A	12	MET	2.0
1	A	17	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 [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($\text{\AA}^2$)	Q<0.9
3	PCR	A	801	8/8	0.91	0.09	31,33,37,38	0
4	EDO	B	901	4/4	0.94	0.09	31,41,41,41	0

6.5 Other polymers [i](#)

There are no such residues in this entry.