



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 15, 2026 – 02:28 PM UTC

PDB ID : 1P35 / pdb_00001p35
Title : CRYSTAL STRUCTURE OF BACULOVIRUS P35
Authors : Fisher, A.J.; Delacruz, W.P.; Zoog, S.J.; Schneider, C.L.; Friesen, P.D.
Deposited on : 1998-09-18
Resolution : 2.20 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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

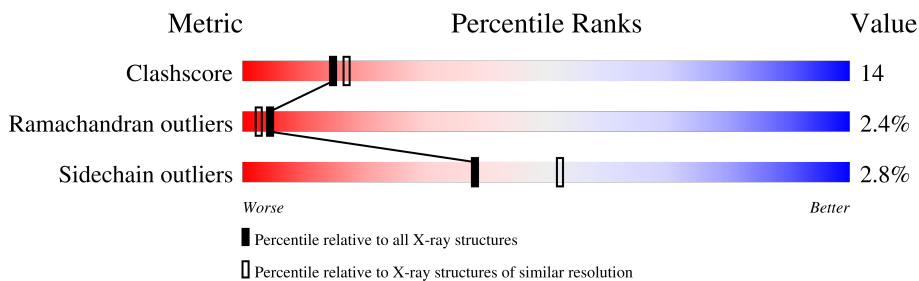
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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))
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	299	 69% 25% 5%
1	B	299	 67% 27% 5% .
1	C	299	 61% 33% . .

2 Entry composition [i](#)

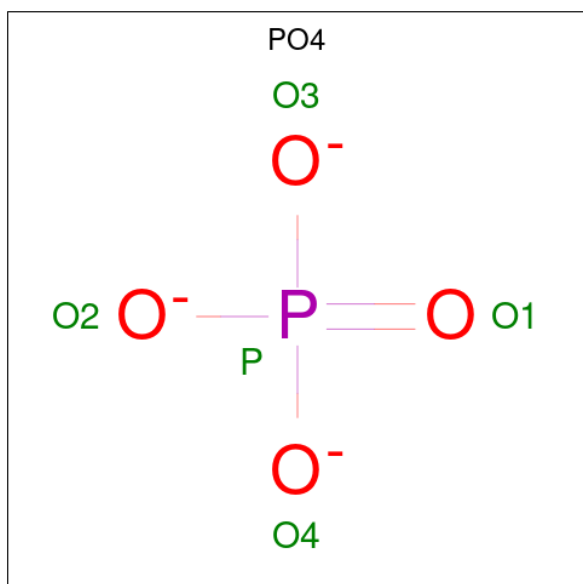
There are 4 unique types of molecules in this entry. The entry contains 7538 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 P35.

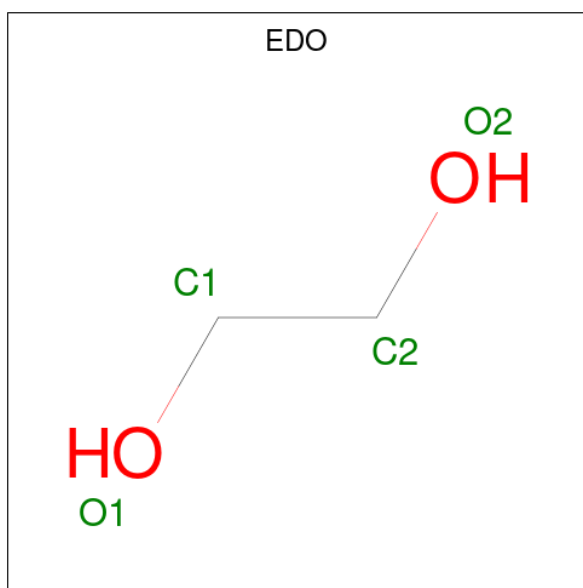
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	299	Total	C	N	O	S	0	0	0
			2416	1544	398	464	10			
1	B	298	Total	C	N	O	S	0	0	0
			2438	1559	400	468	11			
1	C	295	Total	C	N	O	S	0	0	0
			2390	1526	393	460	11			

- Molecule 2 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



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

- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



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	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is water.

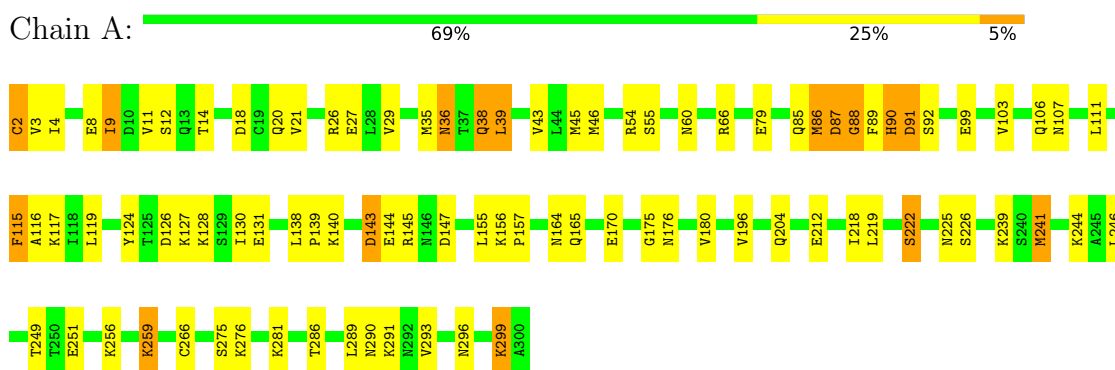
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	94	Total	O	0	0
			94	94		
4	B	105	Total	O	0	0
			105	105		
4	C	68	Total	O	0	0
			68	68		

3 Residue-property plots [i](#)

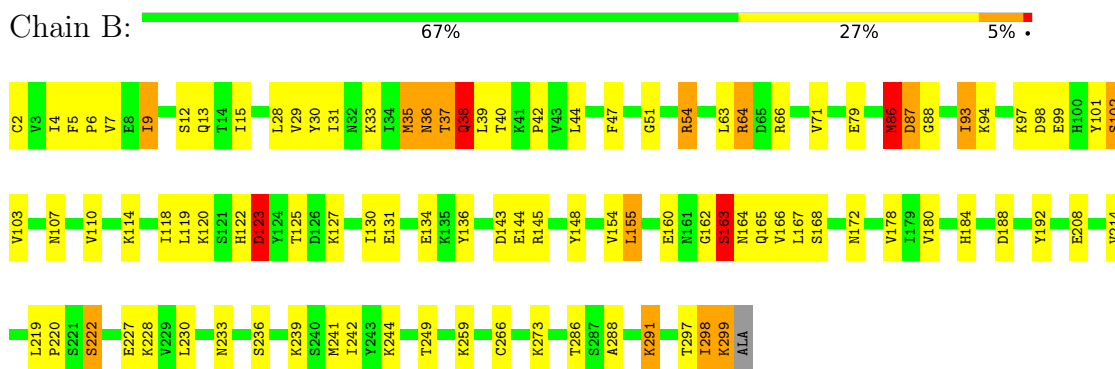
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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.

Note EDS was not executed.

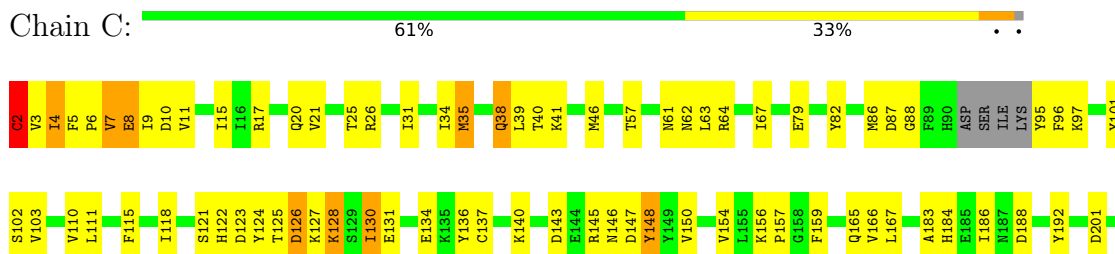
• Molecule 1: P35

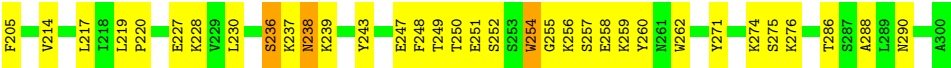


• Molecule 1: P35



• Molecule 1: P35





4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	114.58Å 130.11Å 181.08Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.20	Depositor
% Data completeness (in resolution range)	97.6 (30.00-2.20)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 0.3	Depositor
R, R_{free}	0.196 , 0.262	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7538	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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

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	0.98	3/2464 (0.1%)	1.32	30/3328 (0.9%)
1	B	1.05	5/2488 (0.2%)	1.34	29/3356 (0.9%)
1	C	0.91	0/2435	1.26	27/3283 (0.8%)
All	All	0.99	8/7387 (0.1%)	1.30	86/9967 (0.9%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	86	MET	C-O	8.58	1.34	1.24
1	B	86	MET	SD-CE	7.66	1.98	1.79
1	A	86	MET	N-CA	7.17	1.55	1.46
1	B	299	LYS	CE-NZ	6.53	1.69	1.49
1	B	35	MET	SD-CE	6.01	1.94	1.79
1	B	71	VAL	CA-CB	5.89	1.61	1.54
1	B	86	MET	CG-SD	5.25	1.93	1.80
1	A	256	LYS	CA-C	5.09	1.55	1.52

All (86) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	236	SER	N-CA-C	-9.88	99.54	114.16
1	A	299	LYS	N-CA-C	9.65	123.17	111.40
1	C	41	LYS	CA-C-N	9.53	131.75	119.84
1	C	41	LYS	C-N-CA	9.53	131.75	119.84
1	A	90	HIS	N-CA-C	9.23	123.95	108.90
1	A	156	LYS	CA-C-N	9.19	129.39	119.28
1	A	156	LYS	C-N-CA	9.19	129.39	119.28
1	C	63	LEU	N-CA-C	-8.96	101.42	111.82
1	B	79	GLU	N-CA-C	8.48	123.81	110.32
1	B	9	ILE	N-CA-C	-8.24	98.84	109.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	222	SER	N-CA-C	-8.09	102.44	112.88
1	A	180	VAL	N-CA-C	-8.04	100.25	107.56
1	A	115	PHE	N-CA-C	7.96	119.59	111.07
1	A	35	MET	N-CA-C	7.87	122.88	113.28
1	B	291	LYS	N-CA-C	7.61	120.74	109.24
1	A	157	PRO	N-CA-C	7.26	123.45	113.65
1	B	13	GLN	N-CA-C	7.11	120.69	110.24
1	B	7	VAL	CA-C-N	-7.03	112.70	123.17
1	B	7	VAL	C-N-CA	-7.03	112.70	123.17
1	B	298	ILE	CB-CA-C	-7.03	101.54	111.38
1	B	188	ASP	N-CA-C	7.01	118.92	111.28
1	A	21	VAL	N-CA-C	-7.00	105.79	111.81
1	B	136	TYR	N-CA-C	6.96	122.06	113.50
1	A	259	LYS	N-CA-C	6.95	119.53	110.43
1	A	103	VAL	N-CA-C	6.79	117.68	108.17
1	B	144	GLU	N-CA-C	-6.50	104.60	112.54
1	A	111	LEU	N-CA-C	6.43	118.29	111.28
1	C	250	THR	N-CA-C	-6.26	99.90	109.41
1	A	89	PHE	CA-C-N	-6.24	114.19	122.99
1	A	89	PHE	C-N-CA	-6.24	114.19	122.99
1	A	175	GLY	N-CA-C	6.20	127.88	113.18
1	C	39	LEU	N-CA-C	6.20	119.99	110.20
1	C	79	GLU	N-CA-C	6.19	120.02	110.42
1	C	97	LYS	N-CA-C	-6.17	102.57	110.53
1	C	188	ASP	N-CA-C	6.16	120.06	112.54
1	B	4	ILE	N-CA-C	6.07	117.33	108.53
1	B	29	VAL	N-CA-C	-6.03	99.67	108.11
1	C	126	ASP	N-CA-C	6.00	118.97	110.50
1	B	103	VAL	N-CA-C	6.00	117.23	108.53
1	C	110	VAL	N-CA-C	5.95	116.69	110.62
1	C	4	ILE	N-CA-C	5.83	116.99	108.53
1	B	236	SER	N-CA-C	-5.83	100.55	109.65
1	B	7	VAL	N-CA-C	5.82	119.21	111.17
1	B	288	ALA	N-CA-C	-5.81	106.15	113.18
1	C	103	VAL	N-CA-C	5.79	116.81	108.48
1	B	180	VAL	N-CA-C	-5.78	101.92	107.76
1	B	38	GLN	N-CA-C	5.78	123.11	110.80
1	C	2	CYS	CA-CB-SG	-5.76	101.15	114.40
1	C	125	THR	N-CA-C	5.74	119.47	112.23
1	C	166	VAL	N-CA-C	5.69	117.61	108.85
1	B	163	SER	N-CA-C	5.67	118.90	110.52
1	A	91	ASP	N-CA-C	5.59	122.72	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	156	LYS	CA-C-N	5.58	125.58	119.89
1	C	156	LYS	C-N-CA	5.58	125.58	119.89
1	B	123	ASP	N-CA-C	5.58	120.04	113.23
1	A	3	VAL	N-CA-C	-5.56	98.65	107.15
1	B	233	ASN	N-CA-C	-5.55	96.72	107.44
1	A	2	CYS	CA-CB-SG	-5.55	101.63	114.40
1	C	25	THR	N-CA-C	5.49	118.40	109.24
1	A	293	VAL	N-CA-C	-5.44	100.55	108.17
1	B	273	LYS	N-CA-C	5.44	117.96	111.71
1	A	29	VAL	N-CA-C	-5.42	100.53	108.11
1	A	291	LYS	N-CA-C	5.41	117.29	109.07
1	A	36	ASN	N-CA-C	5.40	118.27	110.28
1	C	21	VAL	N-CA-C	-5.38	107.18	111.81
1	C	130	ILE	N-CA-C	5.37	116.75	110.62
1	B	123	ASP	CA-C-N	-5.36	115.87	122.84
1	B	123	ASP	C-N-CA	-5.36	115.87	122.84
1	A	164	ASN	N-CA-C	-5.34	101.77	110.20
1	B	299	LYS	N-CA-C	-5.32	96.10	111.00
1	B	162	GLY	N-CA-C	-5.30	107.30	115.73
1	A	107	ASN	N-CA-C	-5.29	102.44	110.28
1	A	4	ILE	N-CA-C	5.28	116.57	108.71
1	A	79	GLU	N-CA-C	5.26	118.31	110.52
1	A	226	SER	N-CA-C	5.25	118.82	112.93
1	C	137	CYS	N-CA-C	5.18	117.92	111.24
1	B	102	SER	N-CA-C	-5.17	100.30	108.73
1	A	117	LYS	N-CA-C	-5.16	105.55	111.07
1	C	217	LEU	N-CA-C	5.14	118.32	110.20
1	C	150	VAL	N-CA-C	5.14	115.37	107.77
1	A	219	LEU	N-CA-C	5.13	117.23	110.36
1	C	10	ASP	N-CA-C	5.12	117.25	108.90
1	C	288	ALA	N-CA-C	-5.12	105.78	112.23
1	B	166	VAL	N-CA-C	5.11	116.97	108.99
1	A	222	SER	N-CA-C	-5.08	106.77	113.17
1	C	57	THR	N-CA-C	5.04	116.95	109.69

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	2416	0	2367	62	0
1	B	2438	0	2412	74	0
1	C	2390	0	2360	67	0
2	A	10	0	0	0	0
2	B	5	0	0	0	0
3	A	8	0	12	0	0
3	B	4	0	6	0	0
4	A	94	0	0	2	0
4	B	105	0	0	4	0
4	C	68	0	0	3	0
All	All	7538	0	7157	199	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 (199) 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:299:LYS:CE	1:B:299:LYS:NZ	1.68	1.55
1:B:9:ILE:HA	1:B:36:ASN:OD1	1.47	1.12
1:A:38:GLN:HG2	1:A:39:LEU:H	1.11	1.07
1:C:128:LYS:HA	1:C:128:LYS:HE2	1.50	0.92
1:A:60:ASN:HD21	1:A:66:ARG:HH22	0.92	0.89
1:A:251:GLU:HG2	1:A:259:LYS:NZ	1.90	0.87
1:A:36:ASN:HD22	1:A:38:GLN:NE2	1.72	0.87
1:A:8:GLU:HG3	1:A:9:ILE:H	1.41	0.85
1:A:38:GLN:HG2	1:A:39:LEU:N	1.93	0.84
1:A:60:ASN:HD21	1:A:66:ARG:NH2	1.75	0.84
1:B:114:LYS:O	1:B:118:ILE:HG13	1.81	0.80
1:A:90:HIS:O	1:A:92:SER:N	2.15	0.78
1:C:228:LYS:HE2	4:C:317:HOH:O	1.82	0.78
1:B:86:MET:HE2	1:B:87:ASP:H	1.50	0.74
1:B:134:GLU:OE1	1:C:145:ARG:HD2	1.87	0.74
1:A:60:ASN:ND2	1:A:66:ARG:HH22	1.78	0.73
1:B:298:ILE:HG22	1:B:299:LYS:N	2.03	0.73
1:A:8:GLU:HG3	1:A:9:ILE:N	2.02	0.73
1:B:2:CYS:HB2	1:B:30:TYR:OH	1.90	0.71
1:A:251:GLU:HG2	1:A:259:LYS:HZ1	1.54	0.71
1:B:37:THR:OG1	1:B:38:GLN:HG3	1.90	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:36:ASN:HD22	1:A:38:GLN:HE22	1.37	0.70
1:C:128:LYS:HA	1:C:128:LYS:CE	2.20	0.70
1:B:102:SER:HB3	1:B:154:VAL:HG23	1.74	0.70
1:B:33:LYS:HE2	1:B:163:SER:O	1.91	0.69
1:A:143:ASP:O	1:A:145:ARG:N	2.26	0.69
1:A:251:GLU:HG2	1:A:259:LYS:HZ3	1.59	0.68
1:A:55:SER:HB3	1:C:256:LYS:HE2	1.74	0.68
1:A:204:GLN:HE22	1:A:299:LYS:HE2	1.58	0.68
1:C:38:GLN:H	1:C:38:GLN:CD	2.02	0.67
1:A:8:GLU:CG	1:A:9:ILE:H	2.08	0.66
1:C:140:LYS:HA	1:C:140:LYS:HE2	1.76	0.66
1:C:35:MET:HA	1:C:35:MET:HE2	1.79	0.65
1:A:18:ASP:HA	1:A:27:GLU:O	1.97	0.65
1:C:101:TYR:CE1	1:C:165:GLN:HB3	2.32	0.65
1:A:249:THR:HG21	1:A:259:LYS:HD3	1.79	0.64
1:B:102:SER:HB3	1:B:154:VAL:CG2	2.29	0.63
1:A:85:GLN:C	1:A:87:ASP:H	2.06	0.63
1:C:122:HIS:O	1:C:123:ASP:HB2	1.99	0.62
1:C:143:ASP:HB3	4:C:338:HOH:O	2.00	0.62
1:A:38:GLN:CG	1:A:39:LEU:H	1.96	0.61
1:A:87:ASP:CG	1:A:88:GLY:N	2.58	0.61
1:A:204:GLN:NE2	1:A:299:LYS:HE2	2.15	0.61
1:A:36:ASN:ND2	1:A:38:GLN:HE22	1.97	0.61
1:B:291:LYS:HE3	4:B:349:HOH:O	1.99	0.61
1:C:111:LEU:O	1:C:115:PHE:HB3	2.00	0.60
1:B:2:CYS:SG	1:B:47:PHE:HB3	2.41	0.60
1:B:107:ASN:OD1	1:B:110:VAL:HG23	2.01	0.60
1:B:2:CYS:SG	1:B:47:PHE:HD2	2.24	0.60
1:A:54:ARG:NH2	1:A:170:GLU:OE1	2.34	0.60
1:C:147:ASP:O	1:C:148:TYR:O	2.19	0.60
1:A:119:LEU:HD12	1:A:130:ILE:HG12	1.84	0.59
1:B:99:GLU:HB2	1:B:165:GLN:OE1	2.01	0.59
1:C:2:CYS:O	1:C:184:HIS:HA	2.02	0.59
1:C:5:PHE:HA	1:C:6:PRO:C	2.28	0.59
1:A:85:GLN:O	1:A:87:ASP:N	2.36	0.59
1:B:51:GLY:HA3	1:B:172:ASN:O	2.01	0.59
1:A:20:GLN:HA	1:A:26:ARG:HG2	1.84	0.58
1:A:127:LYS:O	1:A:131:GLU:HG3	2.03	0.58
1:C:230:LEU:HD12	1:C:247:GLU:CD	2.28	0.58
1:C:237:LYS:N	1:C:237:LYS:HD2	2.19	0.58
1:B:119:LEU:HD12	1:B:130:ILE:HG12	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:11:VAL:HG22	1:A:12:SER:N	2.20	0.57
1:A:87:ASP:CG	1:A:88:GLY:H	2.13	0.57
1:B:9:ILE:CA	1:B:36:ASN:OD1	2.37	0.56
1:C:34:ILE:H	1:C:165:GLN:NE2	2.03	0.56
1:C:236:SER:C	1:C:237:LYS:HD2	2.30	0.56
1:B:54:ARG:HA	1:B:54:ARG:HE	1.71	0.56
1:A:249:THR:CG2	1:A:259:LYS:HD3	2.36	0.56
1:C:15:ILE:HD12	1:C:64:ARG:HG2	1.88	0.56
1:A:140:LYS:HE2	1:A:290:ASN:ND2	2.21	0.55
1:B:2:CYS:HG	1:B:47:PHE:HD2	1.48	0.54
1:B:93:ILE:HG13	1:B:94:LYS:N	2.22	0.54
1:A:55:SER:HB3	1:C:256:LYS:CE	2.37	0.54
1:C:34:ILE:H	1:C:165:GLN:HE21	1.54	0.54
1:B:178:VAL:HG23	1:B:297:THR:CG2	2.37	0.54
1:C:3:VAL:HB	1:C:46:MET:O	2.08	0.54
1:B:86:MET:C	1:B:88:GLY:H	2.15	0.53
1:B:98:ASP:OD1	1:B:164:ASN:HB2	2.08	0.53
1:C:236:SER:O	1:C:238:ASN:ND2	2.41	0.53
1:A:143:ASP:C	1:A:145:ARG:H	2.15	0.53
1:A:8:GLU:CG	1:A:9:ILE:N	2.70	0.53
1:C:145:ARG:O	1:C:146:ASN:ND2	2.42	0.53
1:B:2:CYS:SG	1:B:47:PHE:CD2	3.01	0.53
1:B:298:ILE:O	1:B:299:LYS:HB2	2.09	0.53
1:B:44:LEU:CD2	1:B:154:VAL:HG12	2.38	0.53
1:A:2:CYS:N	1:A:45:MET:HG3	2.25	0.52
1:A:212:GLU:HG2	1:A:289:LEU:HD11	1.91	0.52
1:B:36:ASN:O	1:B:37:THR:O	2.28	0.52
1:C:192:TYR:O	1:C:286:THR:HA	2.09	0.51
1:B:298:ILE:HG22	1:B:299:LYS:H	1.73	0.51
1:C:40:THR:O	1:C:157:PRO:HG2	2.10	0.51
1:C:126:ASP:OD2	1:C:128:LYS:HB3	2.10	0.51
1:B:214:VAL:HG21	1:B:242:ILE:HG22	1.93	0.51
1:A:85:GLN:C	1:A:87:ASP:N	2.69	0.51
1:A:145:ARG:O	1:A:147:ASP:OD1	2.28	0.51
1:C:258:GLU:CD	1:C:260:TYR:HE1	2.19	0.50
1:A:99:GLU:HB2	1:A:165:GLN:OE1	2.12	0.50
1:C:124:TYR:O	1:C:130:ILE:HD11	2.12	0.50
1:C:5:PHE:CD2	1:C:6:PRO:HA	2.47	0.50
1:C:2:CYS:HB2	1:C:183:ALA:O	2.12	0.49
1:B:298:ILE:CG2	1:B:299:LYS:N	2.73	0.49
1:B:239:LYS:HD2	1:B:241:MET:SD	2.53	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:20:GLN:HA	1:C:26:ARG:HG2	1.94	0.49
1:B:5:PHE:HA	1:B:6:PRO:C	2.38	0.48
1:B:12:SER:HB3	1:B:35:MET:SD	2.53	0.48
1:B:143:ASP:O	1:B:143:ASP:OD1	2.32	0.48
1:B:64:ARG:HH11	1:B:64:ARG:HG3	1.79	0.48
1:C:249:THR:HG21	1:C:259:LYS:CE	2.43	0.48
1:B:97:LYS:O	1:B:163:SER:OG	2.28	0.48
1:C:146:ASN:HB2	4:C:338:HOH:O	2.13	0.47
1:C:82:TYR:HB2	1:C:262:TRP:CZ2	2.50	0.47
1:B:33:LYS:HE2	1:B:163:SER:C	2.39	0.47
1:A:126:ASP:OD2	1:A:128:LYS:HB3	2.13	0.47
1:B:86:MET:HE2	1:B:87:ASP:N	2.25	0.47
1:B:131:GLU:HB3	1:C:145:ARG:HG2	1.96	0.47
1:C:127:LYS:O	1:C:131:GLU:HG3	2.14	0.47
1:B:102:SER:O	1:B:154:VAL:HG22	2.15	0.47
1:C:256:LYS:O	1:C:258:GLU:N	2.46	0.47
1:B:249:THR:HG21	1:B:259:LYS:HD3	1.97	0.46
1:A:2:CYS:N	1:A:45:MET:CG	2.78	0.46
1:C:95:TYR:O	1:C:96:PHE:HB2	2.15	0.46
1:B:127:LYS:O	1:B:131:GLU:HG3	2.15	0.46
1:C:118:ILE:O	1:C:121:SER:OG	2.30	0.46
1:B:15:ILE:HB	1:B:31:ILE:HB	1.96	0.46
1:C:236:SER:HB2	1:C:239:LYS:HB3	1.98	0.46
1:A:14:THR:O	1:A:196:VAL:HA	2.16	0.46
1:A:275:SER:O	1:A:276:LYS:HB2	2.16	0.46
1:C:140:LYS:HD2	1:C:290:ASN:ND2	2.30	0.46
1:C:249:THR:HG21	1:C:259:LYS:HE2	1.98	0.46
1:C:205:PHE:HB2	1:C:271:TYR:CE2	2.51	0.46
1:C:159:PHE:CD1	1:C:159:PHE:C	2.94	0.45
1:B:2:CYS:CB	1:B:30:TYR:OH	2.63	0.45
1:B:148:TYR:HA	4:B:390:HOH:O	2.15	0.45
1:A:244:LYS:O	1:A:266:CYS:HA	2.16	0.45
1:C:251:GLU:HB3	1:C:259:LYS:HG2	1.99	0.45
1:A:143:ASP:C	1:A:145:ARG:N	2.75	0.45
1:C:35:MET:HA	1:C:35:MET:CE	2.47	0.45
1:A:106:GLN:NE2	1:A:106:GLN:HA	2.31	0.45
1:A:239:LYS:C	1:A:241:MET:HE2	2.41	0.44
1:A:11:VAL:CG2	1:A:12:SER:N	2.80	0.44
1:B:222:SER:N	1:B:227:GLU:OE2	2.41	0.44
1:C:6:PRO:C	1:C:8:GLU:H	2.26	0.44
1:B:66:ARG:HB3	1:B:66:ARG:NH1	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:6:PRO:HG2	1:C:9:ILE:HG13	2.00	0.44
1:B:244:LYS:O	1:B:266:CYS:HA	2.18	0.44
1:A:138:LEU:N	1:A:139:PRO:CD	2.81	0.43
1:B:127:LYS:HE2	1:B:131:GLU:OE1	2.18	0.43
1:B:28:LEU:O	1:B:168:SER:HA	2.18	0.43
1:B:228:LYS:HD2	1:B:228:LYS:HA	1.76	0.43
1:C:130:ILE:HD12	1:C:130:ILE:N	2.33	0.43
1:A:218:ILE:HB	1:A:286:THR:OG1	2.18	0.43
1:B:160:GLU:O	1:B:163:SER:HB2	2.18	0.43
1:C:136:TYR:O	1:C:186:ILE:HG13	2.18	0.43
1:A:115:PHE:CD1	1:A:116:ALA:N	2.87	0.43
1:C:201:ASP:OD1	1:C:201:ASP:C	2.61	0.43
1:B:44:LEU:HD22	1:B:154:VAL:HG12	2.01	0.42
1:C:102:SER:HB3	1:C:154:VAL:HB	2.01	0.42
1:B:6:PRO:O	1:B:9:ILE:HG12	2.19	0.42
1:B:155:LEU:HD21	1:B:165:GLN:HG3	1.99	0.42
1:B:42:PRO:HG2	4:B:344:HOH:O	2.18	0.42
1:C:17:ARG:HB2	1:C:67:ILE:HD13	2.01	0.42
1:B:119:LEU:CD1	1:B:130:ILE:HG12	2.47	0.42
1:B:122:HIS:O	1:B:123:ASP:HB2	2.20	0.42
1:B:219:LEU:HB3	1:B:220:PRO:HD2	2.02	0.42
1:C:219:LEU:HB3	1:C:220:PRO:HD2	2.02	0.42
1:A:46:MET:HG3	4:A:314:HOH:O	2.18	0.42
1:C:214:VAL:HG11	1:C:243:TYR:HA	2.01	0.42
1:A:43:VAL:HB	1:A:155:LEU:HB3	2.01	0.42
1:B:167:LEU:C	1:B:167:LEU:HD12	2.43	0.42
1:B:120:LYS:HG2	1:B:125:THR:HG22	2.02	0.42
1:A:119:LEU:HB3	1:A:124:TYR:HB2	2.02	0.42
1:B:86:MET:C	1:B:88:GLY:N	2.77	0.42
1:B:208:GLU:HG3	4:B:327:HOH:O	2.20	0.42
1:B:37:THR:OG1	1:B:38:GLN:N	2.49	0.42
1:B:127:LYS:HE2	1:B:131:GLU:CD	2.45	0.42
1:B:192:TYR:O	1:B:286:THR:HA	2.20	0.41
1:B:54:ARG:HE	1:B:54:ARG:CA	2.31	0.41
1:A:115:PHE:CD1	1:A:115:PHE:C	2.99	0.41
1:A:225:ASN:ND2	1:A:225:ASN:C	2.76	0.41
1:A:176:ASN:O	1:A:296:ASN:HA	2.21	0.41
1:C:252:SER:C	1:C:254:TRP:H	2.29	0.41
1:B:37:THR:H	1:B:37:THR:HG23	1.41	0.41
1:C:127:LYS:HG2	1:C:131:GLU:OE2	2.20	0.41
1:C:31:ILE:HG21	1:C:64:ARG:HG3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:275:SER:O	1:C:276:LYS:HB2	2.21	0.41
1:A:204:GLN:HE22	1:A:299:LYS:CE	2.29	0.41
1:A:222:SER:HB3	1:A:246:LEU:HD21	2.01	0.41
1:B:178:VAL:HG23	1:B:297:THR:HG22	2.02	0.41
1:B:192:TYR:CD1	1:B:192:TYR:N	2.89	0.41
1:B:38:GLN:HG3	1:B:38:GLN:H	1.47	0.40
1:A:281:LYS:HE3	4:A:335:HOH:O	2.21	0.40
1:C:134:GLU:O	1:C:134:GLU:CG	2.70	0.40
1:C:4:ILE:HD12	1:C:11:VAL:HG11	2.03	0.40
1:C:130:ILE:N	1:C:130:ILE:CD1	2.85	0.40
1:B:101:TYR:CE1	1:B:165:GLN:HB3	2.57	0.40
1:C:7:VAL:HG11	1:C:136:TYR:HB2	2.04	0.40
1:C:167:LEU:HD12	1:C:167:LEU:C	2.47	0.40
1:C:227:GLU:HA	1:C:248:PHE:HB3	2.03	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	297/299 (99%)	272 (92%)	17 (6%)	8 (3%)	4	2
1	B	296/299 (99%)	283 (96%)	8 (3%)	5 (2%)	7	5
1	C	291/299 (97%)	266 (91%)	17 (6%)	8 (3%)	4	2
All	All	884/897 (99%)	821 (93%)	42 (5%)	21 (2%)	4	3

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	9	ILE
1	A	39	LEU
1	A	86	MET

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Mol	Chain	Res	Type
1	A	87	ASP
1	A	91	ASP
1	A	144	GLU
1	B	37	THR
1	B	38	GLN
1	B	145	ARG
1	C	86	MET
1	C	148	TYR
1	C	238	ASN
1	A	38	GLN
1	A	88	GLY
1	B	36	ASN
1	B	87	ASP
1	C	254	TRP
1	C	257	SER
1	C	88	GLY
1	C	7	VAL
1	C	255	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	271/280 (97%)	269 (99%)	2 (1%)	76	87
1	B	279/280 (100%)	267 (96%)	12 (4%)	26	35
1	C	271/280 (97%)	262 (97%)	9 (3%)	33	45
All	All	821/840 (98%)	798 (97%)	23 (3%)	38	52

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	143	ASP
1	A	241	MET
1	B	39	LEU
1	B	40	THR

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Mol	Chain	Res	Type
1	B	54	ARG
1	B	63	LEU
1	B	64	ARG
1	B	86	MET
1	B	93	ILE
1	B	123	ASP
1	B	155	LEU
1	B	163	SER
1	B	184	HIS
1	B	230	LEU
1	C	2	CYS
1	C	8	GLU
1	C	35	MET
1	C	38	GLN
1	C	61	ASN
1	C	62	ASN
1	C	87	ASP
1	C	128	LYS
1	C	274	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	36	ASN
1	A	74	GLN
1	A	90	HIS
1	A	106	GLN
1	A	161	ASN
1	A	204	GLN
1	A	225	ASN
1	A	261	ASN
1	A	284	ASN
1	B	24	GLN
1	B	48	ASN
1	B	106	GLN
1	B	172	ASN
1	B	238	ASN
1	B	261	ASN
1	B	284	ASN
1	C	24	GLN
1	C	62	ASN
1	C	106	GLN

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Mol	Chain	Res	Type
1	C	146	ASN
1	C	165	GLN
1	C	215	GLN

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 ⓘ

6 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	$\# Z > 2$
2	PO4	B	301	-	4,4,4	1.07	0	6,6,6	0.68	0
3	EDO	A	302	-	3,3,3	0.44	0	2,2,2	0.43	0
3	EDO	B	302	-	3,3,3	0.51	0	2,2,2	0.34	0
2	PO4	A	301	-	4,4,4	0.78	0	6,6,6	0.79	0
2	PO4	A	1	-	4,4,4	0.96	0	6,6,6	0.70	0
3	EDO	A	303	-	3,3,3	0.48	0	2,2,2	0.38	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	302	-	-	1/1/1/1	-
3	EDO	B	302	-	-	1/1/1/1	-
3	EDO	A	303	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	302	EDO	O1-C1-C2-O2
3	A	302	EDO	O1-C1-C2-O2

There are no ring outliers.

No monomer is involved in short contacts.

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 [i](#)

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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section is therefore empty.

6.4 Ligands [i](#)

EDS was not executed - this section is therefore empty.

6.5 Other polymers [i](#)

EDS was not executed - this section is therefore empty.