



Full wwPDB X-ray Structure Validation Report ⓘ

May 19, 2020 – 03:06 am BST

PDB ID : 2HOY
Title : Inter-subunit signaling in GSAM
Authors : Stetefeld, J.
Deposited on : 2006-07-17
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

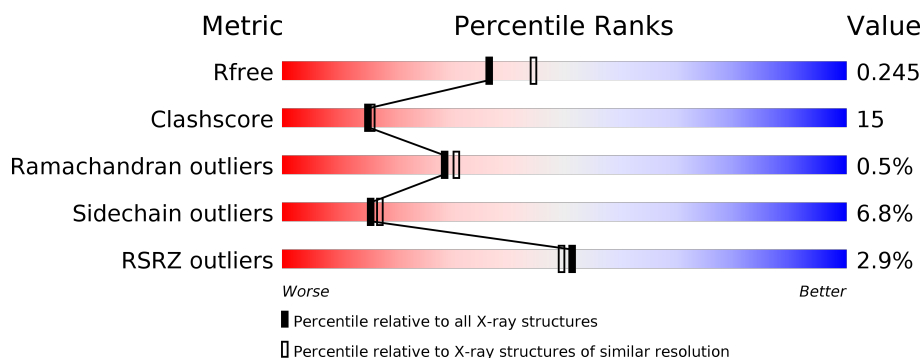
1 Overall quality at a glance

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))
R_{free}	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (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 on 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	432	<div> <div>2%</div> <div> <div></div> <div>67%</div> <div>23%</div> <div>•</div> <div>7%</div> </div> </div>
1	B	432	<div> <div>3%</div> <div> <div></div> <div>67%</div> <div>21%</div> <div>•</div> <div>9%</div> </div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6601 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 Glutamate-1-semialdehyde 2,1-aminomutase (GSAM) apo-form.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	402	Total	C	N	O	S	0	0	0
			3033	1933	507	574	19			
1	B	393	Total	C	N	O	S	0	0	0
			2965	1892	494	562	17			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	108	ASN	ILE	CONFLICT	UNP P24630
A	133	ILE	LEU	CONFLICT	UNP P24630
A	172	SER	ASP	CONFLICT	UNP P24630
A	179	LYS	SER	CONFLICT	UNP P24630
A	187	THR	ALA	CONFLICT	UNP P24630
A	327	GLY	ALA	CONFLICT	UNP P24630
B	108	ASN	ILE	CONFLICT	UNP P24630
B	133	ILE	LEU	CONFLICT	UNP P24630
B	172	SER	ASP	CONFLICT	UNP P24630
B	179	LYS	SER	CONFLICT	UNP P24630
B	187	THR	ALA	CONFLICT	UNP P24630
B	327	GLY	ALA	CONFLICT	UNP P24630

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



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

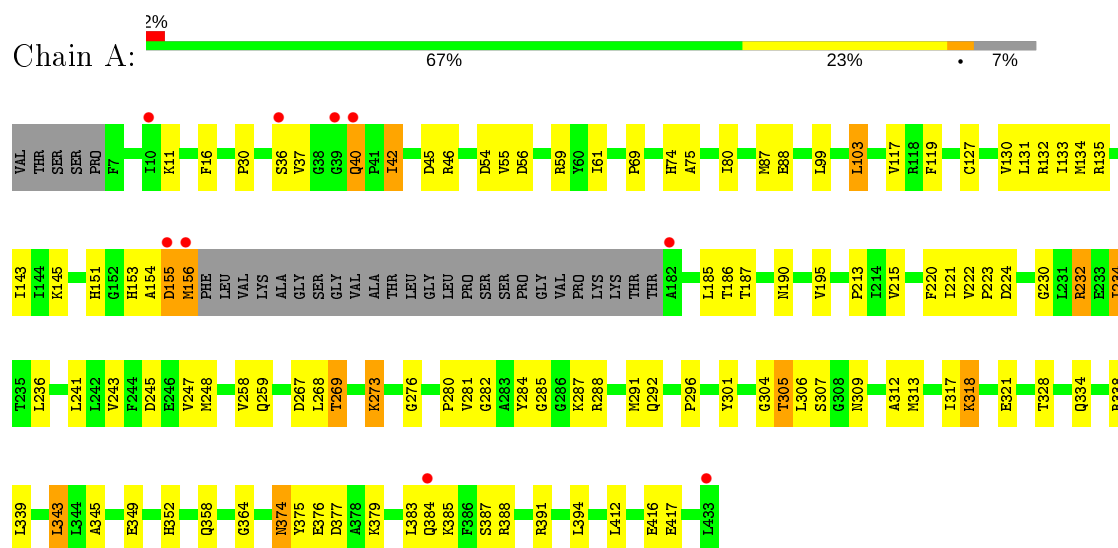
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	316	Total	O	0	0
			316	316		
3	B	277	Total	O	0	0
			277	277		

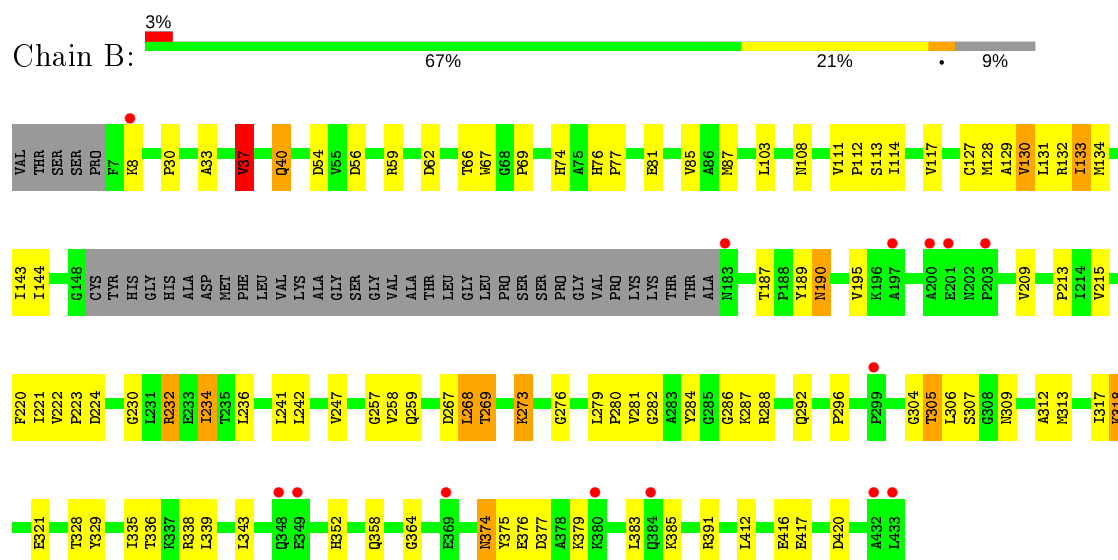
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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: Glutamate-1-semialdehyde 2,1-aminomutase (GSAM) apo-form



- Molecule 1: Glutamate-1-semialdehyde 2,1-aminomutase (GSAM) apo-form



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	65.99Å 107.08Å 122.05Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.40 – 2.20 23.77 – 2.20	Depositor EDS
% Data completeness (in resolution range)	93.7 (19.40-2.20) 93.8 (23.77-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.40 (at 2.19Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.220 , 0.248 0.218 , 0.245	Depositor DCC
R_{free} test set	2048 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å ²)	20.1	Xtriage
Anisotropy	0.390	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 63.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	6601	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.02% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.35	0/3097	0.62	1/4191 (0.0%)
1	B	0.34	0/3026	0.61	0/4095
All	All	0.34	0/6123	0.62	1/8286 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	61	ILE	N-CA-C	-5.02	97.45	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	3033	0	2994	100	0
1	B	2965	0	2940	95	0
2	A	5	0	0	1	0
2	B	5	0	0	0	0
3	A	316	0	0	8	0
3	B	277	0	0	6	0
All	All	6601	0	5934	179	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 15.

All (179) 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:40:GLN:HE21	1:A:40:GLN:HA	1.32	0.95
1:A:338:ARG:HH21	1:A:416:GLU:HG3	1.38	0.88
1:B:190:ASN:HD21	1:B:224:ASP:H	1.23	0.84
1:A:40:GLN:NE2	1:A:40:GLN:HA	1.91	0.82
1:A:30:PRO:HA	1:B:296:PRO:HD3	1.64	0.80
1:A:296:PRO:HD3	1:B:30:PRO:HA	1.64	0.80
1:B:267:ASP:OD2	1:B:287:LYS:HE3	1.81	0.79
1:A:133:ILE:HD11	1:A:284:TYR:CE1	2.18	0.78
1:A:288:ARG:O	1:A:292:GLN:HG2	1.84	0.78
1:A:259:GLN:HE22	1:A:269:THR:HG21	1.47	0.78
1:A:305:THR:HG22	1:A:306:LEU:HG	1.65	0.77
1:B:232:ARG:HH12	1:B:267:ASP:CG	1.89	0.77
1:A:338:ARG:NH2	1:A:416:GLU:HG3	2.03	0.72
1:A:155:ASP:OD1	1:B:132:ARG:HD2	1.89	0.71
1:B:131:LEU:HA	1:B:134:MET:HE3	1.71	0.71
1:B:305:THR:HG22	1:B:306:LEU:HG	1.72	0.71
1:A:190:ASN:HD21	1:A:224:ASP:H	1.39	0.70
1:B:67:TRP:O	1:B:273:LYS:HE3	1.91	0.70
1:B:40:GLN:HE21	1:B:40:GLN:HA	1.57	0.69
1:B:259:GLN:HE22	1:B:269:THR:HG21	1.56	0.69
1:A:133:ILE:HD11	1:A:284:TYR:HE1	1.57	0.69
1:A:131:LEU:HA	1:A:134:MET:HE3	1.75	0.68
1:A:273:LYS:NZ	1:B:305:THR:HG21	2.08	0.68
1:B:222:VAL:HG13	1:B:223:PRO:HD2	1.74	0.68
1:A:305:THR:HG21	1:B:273:LYS:HZ2	1.59	0.68
1:B:338:ARG:HH22	1:B:416:GLU:HG3	1.59	0.67
1:B:131:LEU:HD23	1:B:134:MET:CE	2.24	0.67
1:A:281:VAL:HG22	1:A:312:ALA:HB1	1.76	0.67
1:A:153:HIS:CD2	1:B:132:ARG:HH12	2.14	0.66
1:A:131:LEU:HD23	1:A:134:MET:HE3	1.78	0.66
1:B:133:ILE:HD11	1:B:284:TYR:CE1	2.31	0.65
1:A:222:VAL:HG13	1:A:223:PRO:HD2	1.78	0.65
1:A:305:THR:HG21	1:B:273:LYS:NZ	2.10	0.65
1:A:195:VAL:HG12	1:A:234:ILE:HD11	1.79	0.64
1:B:131:LEU:HA	1:B:134:MET:CE	2.27	0.64
1:B:127:CYS:HB3	3:B:725:HOH:O	1.99	0.63
1:B:54:ASP:HB3	1:B:56:ASP:H	1.64	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:230:GLY:O	1:B:234:ILE:HG23	1.99	0.62
1:A:318:LYS:HE3	1:A:318:LYS:HA	1.81	0.62
1:A:37:VAL:HG23	1:A:387:SER:HA	1.82	0.61
1:B:190:ASN:ND2	1:B:224:ASP:H	1.96	0.61
1:B:338:ARG:NH2	1:B:416:GLU:HG3	2.16	0.60
1:A:267:ASP:OD2	1:A:287:LYS:HE3	2.00	0.60
1:A:16:PHE:HD2	1:A:40:GLN:HE22	1.49	0.59
1:A:131:LEU:HD23	1:A:134:MET:CE	2.31	0.59
1:B:281:VAL:HG12	1:B:282:GLY:N	2.16	0.59
1:B:317:ILE:O	1:B:321:GLU:HG3	2.03	0.59
1:A:213:PRO:HB2	1:A:258:VAL:HG11	1.85	0.58
1:A:135:ARG:NH1	1:A:156:MET:HG2	2.19	0.58
3:A:678:HOH:O	1:B:74:HIS:HD2	1.85	0.58
1:B:232:ARG:HD2	1:B:236:LEU:CD1	2.34	0.58
1:B:288:ARG:O	1:B:292:GLN:HG2	2.04	0.58
1:A:309:ASN:O	1:A:313:MET:HG2	2.04	0.58
1:B:37:VAL:HG13	1:B:37:VAL:O	2.02	0.57
1:A:230:GLY:O	1:A:234:ILE:HG23	2.04	0.57
1:B:281:VAL:HG22	1:B:312:ALA:HB1	1.86	0.57
1:A:281:VAL:CG2	1:A:312:ALA:HB1	2.35	0.56
1:A:54:ASP:HB3	1:A:56:ASP:H	1.70	0.56
1:B:215:VAL:HB	1:B:221:ILE:HB	1.86	0.56
1:A:69:PRO:HG3	1:A:273:LYS:HB3	1.88	0.56
1:A:131:LEU:HD22	1:A:143:ILE:HD12	1.87	0.56
1:B:374:ASN:ND2	1:B:377:ASP:H	2.02	0.56
1:B:131:LEU:HD23	1:B:134:MET:HE1	1.88	0.55
1:B:232:ARG:NH1	1:B:267:ASP:OD2	2.39	0.55
1:A:352:HIS:HD2	1:A:385:LYS:NZ	2.05	0.55
1:A:232:ARG:HH12	1:A:267:ASP:CG	2.10	0.55
1:A:374:ASN:ND2	1:A:377:ASP:H	2.05	0.55
1:B:281:VAL:HG12	1:B:282:GLY:H	1.71	0.54
1:B:213:PRO:HB2	1:B:258:VAL:HG11	1.88	0.54
1:B:108:ASN:OD1	1:B:114:ILE:HG22	2.08	0.54
1:A:281:VAL:HG12	1:A:282:GLY:N	2.23	0.54
1:B:338:ARG:NH1	1:B:420:ASP:OD1	2.41	0.54
1:A:190:ASN:ND2	1:A:224:ASP:H	2.04	0.53
1:B:352:HIS:HD2	1:B:385:LYS:NZ	2.06	0.53
1:A:153:HIS:HD2	1:B:132:ARG:HH12	1.53	0.53
1:A:220:PHE:HB3	1:A:364:GLY:HA3	1.91	0.53
1:A:374:ASN:ND2	1:A:376:GLU:HB3	2.24	0.53
1:A:195:VAL:HG12	1:A:234:ILE:CD1	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:232:ARG:O	1:A:232:ARG:HD3	2.09	0.53
1:A:267:ASP:HA	1:A:287:LYS:HD2	1.91	0.53
1:B:281:VAL:CG2	1:B:312:ALA:HB1	2.39	0.53
1:A:417:GLU:OE1	1:A:417:GLU:N	2.42	0.52
1:B:268:LEU:HD12	1:B:286:GLY:HA3	1.90	0.52
1:B:62:ASP:OD1	1:B:74:HIS:HE1	1.93	0.52
1:B:195:VAL:HG12	1:B:234:ILE:HD11	1.92	0.52
1:B:134:MET:HE3	1:B:143:ILE:HD13	1.92	0.52
1:A:74:HIS:HD2	3:B:637:HOH:O	1.92	0.52
1:B:130:VAL:O	1:B:134:MET:HG3	2.10	0.51
1:B:375:TYR:CD2	1:B:379:LYS:HE2	2.44	0.51
1:A:131:LEU:HA	1:A:134:MET:CE	2.40	0.51
1:B:195:VAL:HG12	1:B:234:ILE:CD1	2.41	0.51
1:A:276:GLY:HA2	1:A:281:VAL:HG21	1.93	0.51
1:A:248:MET:HE3	3:A:634:HOH:O	2.10	0.50
1:A:375:TYR:CD2	1:A:379:LYS:HE2	2.46	0.50
1:B:417:GLU:OE1	1:B:417:GLU:N	2.44	0.50
1:A:99:LEU:HG	3:A:705:HOH:O	2.10	0.50
1:A:154:ALA:HA	1:B:128:MET:HE1	1.93	0.50
1:A:16:PHE:HA	3:A:811:HOH:O	2.11	0.50
1:B:257:GLY:HA3	3:B:665:HOH:O	2.12	0.50
1:B:220:PHE:HB3	1:B:364:GLY:HA3	1.93	0.50
1:B:133:ILE:HD11	1:B:284:TYR:CD1	2.47	0.50
1:A:75:ALA:HB1	1:A:80:ILE:HD11	1.93	0.50
1:A:215:VAL:HB	1:A:221:ILE:HB	1.93	0.50
1:B:304:GLY:HA3	1:B:307:SER:OG	2.13	0.49
1:A:145:LYS:O	1:A:186:THR:HA	2.12	0.49
1:A:11:LYS:HB2	1:A:55:VAL:HG23	1.95	0.49
1:B:113:SER:OG	1:B:269:THR:CG2	2.61	0.49
1:B:195:VAL:CG1	1:B:234:ILE:HD11	2.43	0.49
1:B:374:ASN:ND2	1:B:376:GLU:HB3	2.28	0.49
1:B:189:TYR:O	1:B:190:ASN:HB2	2.12	0.48
1:B:222:VAL:CG1	1:B:223:PRO:HD2	2.42	0.48
1:B:318:LYS:HA	1:B:318:LYS:HE3	1.94	0.48
1:A:232:ARG:HD2	1:A:236:LEU:CD1	2.45	0.47
1:A:151:HIS:HD2	1:A:245:ASP:OD2	1.96	0.47
1:A:87:MET:HE2	1:A:87:MET:HB3	1.57	0.47
1:A:292:GLN:HA	1:A:292:GLN:OE1	2.13	0.47
1:A:374:ASN:HD21	1:A:376:GLU:HB3	1.80	0.47
1:A:328:THR:HG23	1:A:412:LEU:HD21	1.97	0.47
1:B:338:ARG:HD3	3:B:741:HOH:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:296:PRO:HG3	1:B:33:ALA:HB2	1.97	0.46
1:B:247:VAL:HG12	1:B:273:LYS:HD2	1.97	0.46
2:A:601:PO4:O4	1:B:305:THR:HB	2.15	0.46
1:A:334:GLN:HG3	3:A:731:HOH:O	2.15	0.46
1:B:375:TYR:CE2	1:B:379:LYS:HE2	2.51	0.45
1:B:66:THR:HG23	1:B:69:PRO:HD2	1.98	0.45
1:A:232:ARG:C	1:A:232:ARG:HD3	2.35	0.45
1:A:317:ILE:O	1:A:321:GLU:HG3	2.15	0.45
1:B:232:ARG:HD3	1:B:232:ARG:HA	1.60	0.45
1:A:391:ARG:HD3	3:A:752:HOH:O	2.16	0.45
1:A:45:ASP:OD1	1:A:46:ARG:NH1	2.49	0.45
1:B:276:GLY:HA2	1:B:281:VAL:HG21	1.98	0.45
1:B:335:ILE:HG13	1:B:336:THR:N	2.31	0.45
1:B:81:GLU:O	1:B:85:VAL:HG23	2.17	0.45
1:A:42:ILE:HD12	1:A:54:ASP:OD1	2.17	0.45
1:A:153:HIS:HD2	1:B:132:ARG:NH1	2.16	0.44
1:B:144:ILE:HB	1:B:209:VAL:HG22	2.00	0.44
1:A:345:ALA:O	1:A:349:GLU:HG3	2.18	0.44
1:A:195:VAL:CG1	1:A:234:ILE:HD11	2.45	0.44
1:A:132:ARG:NH1	1:A:301:TYR:O	2.50	0.44
1:B:287:LYS:HG3	3:B:867:HOH:O	2.17	0.44
1:A:247:VAL:HG12	1:A:273:LYS:HE2	1.98	0.44
1:A:134:MET:SD	1:A:243:VAL:HG21	2.58	0.44
1:B:279:LEU:O	1:B:281:VAL:HG23	2.17	0.44
1:A:103:LEU:HD13	1:A:119:PHE:CE2	2.52	0.44
1:A:127:CYS:O	1:A:130:VAL:HG12	2.18	0.43
1:B:328:THR:HG22	1:B:329:TYR:N	2.33	0.43
1:A:222:VAL:CG1	1:A:223:PRO:HD2	2.46	0.43
1:A:153:HIS:O	1:B:132:ARG:NH2	2.51	0.43
1:A:285:GLY:HA2	1:A:291:MET:SD	2.59	0.43
1:B:328:THR:HG23	1:B:412:LEU:HD21	2.01	0.43
1:A:281:VAL:HG12	1:A:282:GLY:H	1.84	0.42
1:B:279:LEU:HD12	1:B:279:LEU:N	2.33	0.42
1:A:87:MET:HE1	1:B:87:MET:CE	2.49	0.42
1:A:276:GLY:CA	1:A:281:VAL:HG21	2.49	0.42
1:A:304:GLY:HA3	1:A:307:SER:OG	2.20	0.42
1:B:309:ASN:O	1:B:313:MET:HG2	2.20	0.42
1:B:8:LYS:O	1:B:8:LYS:HG3	2.20	0.42
1:A:130:VAL:O	1:A:134:MET:HG3	2.20	0.42
1:B:276:GLY:CA	1:B:281:VAL:HG21	2.49	0.42
1:B:391:ARG:HA	1:B:391:ARG:HD2	1.87	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:76:HIS:HA	1:B:77:PRO:HD3	1.92	0.42
1:B:338:ARG:HG3	3:B:825:HOH:O	2.19	0.41
1:A:280:PRO:HB2	1:B:280:PRO:HB2	2.02	0.41
1:B:281:VAL:CG1	1:B:282:GLY:N	2.84	0.41
1:A:131:LEU:HD22	1:A:143:ILE:CD1	2.51	0.41
1:B:129:ALA:O	1:B:133:ILE:HG13	2.20	0.41
1:A:87:MET:CE	1:B:87:MET:CE	2.99	0.41
1:B:87:MET:HB3	1:B:87:MET:HE2	1.64	0.41
1:A:154:ALA:O	1:A:155:ASP:C	2.59	0.41
1:A:232:ARG:CD	1:A:232:ARG:O	2.69	0.41
1:B:111:VAL:HA	1:B:112:PRO:HD3	1.92	0.40
1:B:232:ARG:HA	1:B:242:LEU:HD22	2.03	0.40
1:A:343:LEU:HD12	1:A:343:LEU:HA	1.91	0.40
1:A:384:GLN:HG3	1:A:388:ARG:NH2	2.36	0.40
1:A:37:VAL:CG2	1:A:387:SER:HA	2.50	0.40
1:A:394:LEU:HD13	3:A:675:HOH:O	2.21	0.40
1:A:75:ALA:HB1	1:A:80:ILE:CD1	2.51	0.40
1:A:87:MET:CE	1:B:87:MET:HE1	2.52	0.40
1:A:88:GLU:HB2	3:A:703:HOH:O	2.21	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	398/432 (92%)	374 (94%)	22 (6%)	2 (0%)	29	31
1	B	389/432 (90%)	365 (94%)	22 (6%)	2 (0%)	29	31
All	All	787/864 (91%)	739 (94%)	44 (6%)	4 (0%)	29	31

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	273	LYS
1	B	273	LYS
1	A	155	ASP
1	B	37	VAL

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	311/335 (93%)	290 (93%)	21 (7%)	16	17
1	B	305/335 (91%)	284 (93%)	21 (7%)	15	16
All	All	616/670 (92%)	574 (93%)	42 (7%)	16	17

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	SER
1	A	40	GLN
1	A	42	ILE
1	A	59	ARG
1	A	103	LEU
1	A	117	VAL
1	A	156	MET
1	A	185	LEU
1	A	187	THR
1	A	232	ARG
1	A	234	ILE
1	A	241	LEU
1	A	268	LEU
1	A	269	THR
1	A	305	THR
1	A	318	LYS
1	A	339	LEU
1	A	343	LEU
1	A	358	GLN
1	A	374	ASN

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Mol	Chain	Res	Type
1	A	383	LEU
1	B	37	VAL
1	B	40	GLN
1	B	59	ARG
1	B	103	LEU
1	B	117	VAL
1	B	130	VAL
1	B	133	ILE
1	B	187	THR
1	B	190	ASN
1	B	232	ARG
1	B	234	ILE
1	B	241	LEU
1	B	268	LEU
1	B	269	THR
1	B	305	THR
1	B	318	LYS
1	B	339	LEU
1	B	343	LEU
1	B	358	GLN
1	B	374	ASN
1	B	383	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	40	GLN
1	A	58	ASN
1	A	74	HIS
1	A	121	ASN
1	A	151	HIS
1	A	153	HIS
1	A	190	ASN
1	A	352	HIS
1	A	358	GLN
1	A	373	HIS
1	A	374	ASN
1	B	40	GLN
1	B	58	ASN
1	B	74	HIS
1	B	190	ASN
1	B	352	HIS

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Mol	Chain	Res	Type
1	B	373	HIS
1	B	374	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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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	$\# Z > 2$
2	PO4	A	601	-	4,4,4	1.90	3 (75%)	6,6,6	0.44	0
2	PO4	B	602	-	4,4,4	1.90	3 (75%)	6,6,6	0.42	0

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	602	PO4	P-O3	-2.15	1.48	1.54
2	A	601	PO4	P-O4	-2.14	1.48	1.54
2	B	602	PO4	P-O2	-2.14	1.48	1.54
2	A	601	PO4	P-O3	-2.13	1.48	1.54
2	B	602	PO4	P-O4	-2.07	1.48	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	PO4	P-O2	-2.06	1.48	1.54

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	PO4	1	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 ⓘ

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	402/432 (93%)	-0.02	9 (2%) 62 59	11, 23, 44, 63	0
1	B	393/432 (90%)	0.03	14 (3%) 42 41	11, 24, 43, 54	0
All	All	795/864 (92%)	0.00	23 (2%) 51 49	11, 23, 44, 63	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	183	ASN	4.7
1	B	432	ALA	3.9
1	A	156	MET	3.3
1	A	182	ALA	3.2
1	A	36	SER	3.1
1	B	433	LEU	3.0
1	B	348	GLN	2.7
1	A	40	GLN	2.6
1	A	433	LEU	2.6
1	B	203	PRO	2.6
1	A	384	GLN	2.5
1	A	10	ILE	2.5
1	B	200	ALA	2.5
1	B	197	ALA	2.4
1	B	201	GLU	2.4
1	A	39	GLY	2.4
1	B	349	GLU	2.3
1	B	380	LYS	2.2
1	A	155	ASP	2.2
1	B	384	GLN	2.2
1	B	369	GLU	2.1
1	B	299	PRO	2.1
1	B	8	LYS	2.1

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 carbohydrates 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(\AA^2)	Q<0.9
2	PO4	B	602	5/5	0.75	0.26	79,80,80,81	0
2	PO4	A	601	5/5	0.88	0.20	62,62,63,63	0

6.5 Other polymers [i](#)

There are no such residues in this entry.