



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 04:20 PM UTC

PDB ID : 3IFR / pdb_00003ifr
Title : The crystal structure of xylulose kinase from Rhodospirillum rubrum
Authors : Zhang, Z.; Burley, S.K.; Swaminathan, S.; New York SGX Research Center
for Structural Genomics (NYSGXRC)
Deposited on : 2009-07-24
Resolution : 2.30 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

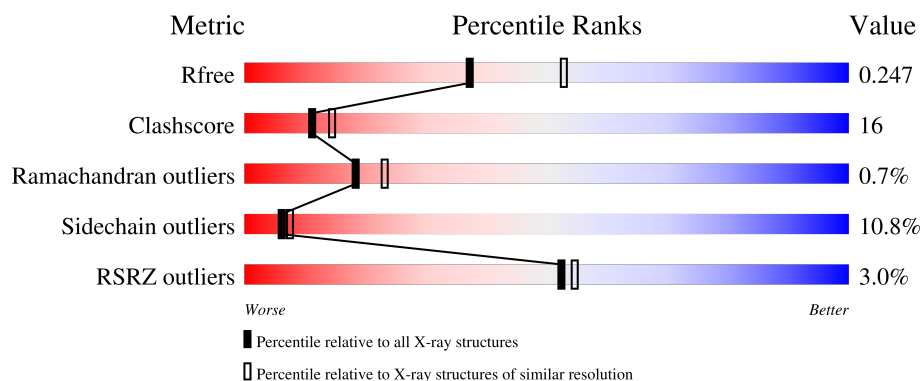
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

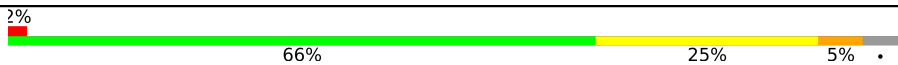
The reported resolution of this entry is 2.30 Å.

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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	508	
1	B	508	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7532 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 Carbohydrate kinase, FGGY.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	488	Total	C	N	O	S	Se	0	0	0
			3624	2301	638	675	5	5			
1	B	480	Total	C	N	O	S	Se	0	0	0
			3564	2263	629	662	5	5			

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	-	expression tag	UNP Q2RUX7
A	2	SER	-	expression tag	UNP Q2RUX7
A	3	LEU	-	expression tag	UNP Q2RUX7
A	501	GLU	-	expression tag	UNP Q2RUX7
A	502	GLY	-	expression tag	UNP Q2RUX7
A	503	HIS	-	expression tag	UNP Q2RUX7
A	504	HIS	-	expression tag	UNP Q2RUX7
A	505	HIS	-	expression tag	UNP Q2RUX7
A	506	HIS	-	expression tag	UNP Q2RUX7
A	507	HIS	-	expression tag	UNP Q2RUX7
A	508	HIS	-	expression tag	UNP Q2RUX7
B	1	MSE	-	expression tag	UNP Q2RUX7
B	2	SER	-	expression tag	UNP Q2RUX7
B	3	LEU	-	expression tag	UNP Q2RUX7
B	501	GLU	-	expression tag	UNP Q2RUX7
B	502	GLY	-	expression tag	UNP Q2RUX7
B	503	HIS	-	expression tag	UNP Q2RUX7
B	504	HIS	-	expression tag	UNP Q2RUX7
B	505	HIS	-	expression tag	UNP Q2RUX7
B	506	HIS	-	expression tag	UNP Q2RUX7
B	507	HIS	-	expression tag	UNP Q2RUX7
B	508	HIS	-	expression tag	UNP Q2RUX7

- 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		

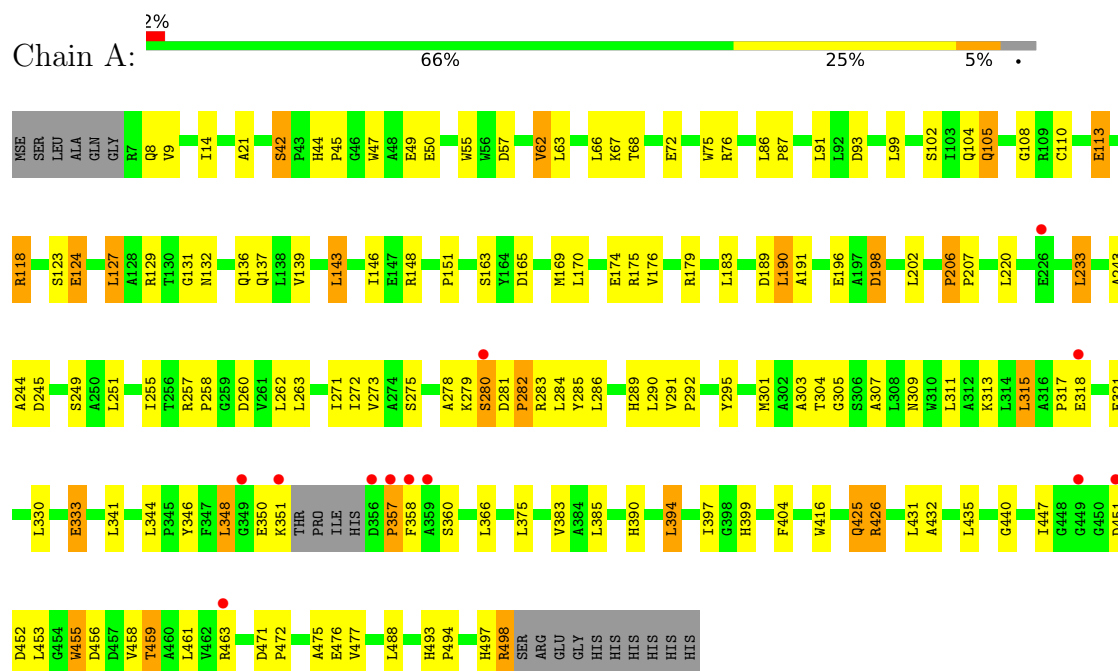
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	170	Total	O	0	0
			170	170		
3	B	169	Total	O	0	0
			169	169		

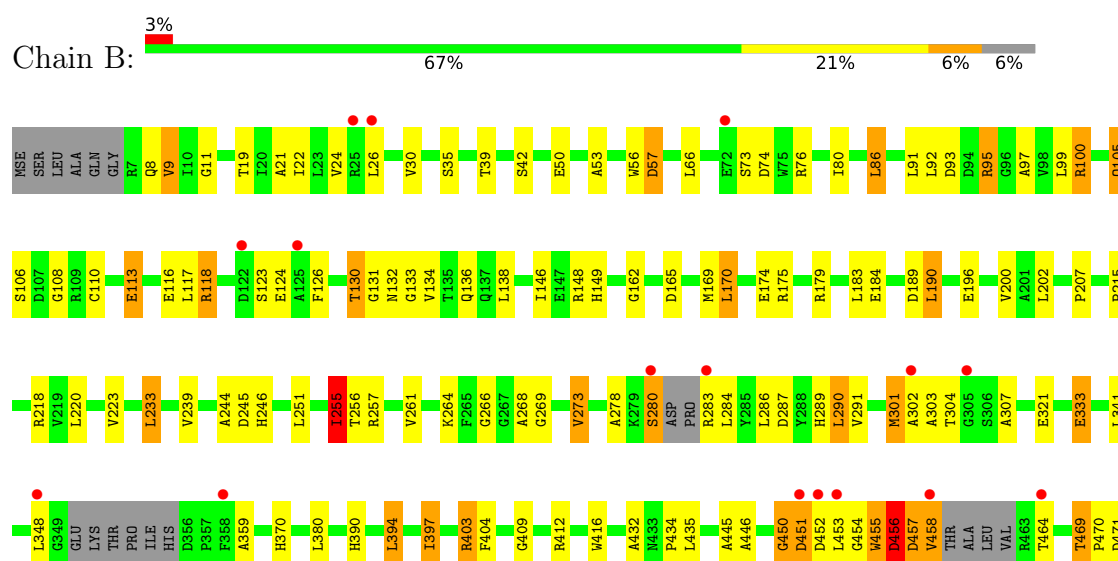
3 Residue-property plots

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: Carbohydrate kinase, FGGY



• Molecule 1: Carbohydrate kinase, FGGY





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	129.09Å 149.81Å 54.94Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	64.55 – 2.30 64.55 – 2.30	Depositor EDS
% Data completeness (in resolution range)	95.8 (64.55-2.30) 98.4 (64.55-2.30)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.05 (at 2.29Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.206 , 0.260 0.204 , 0.247	Depositor DCC
R_{free} test set	2405 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	27.7	Xtriage
Anisotropy	0.678	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 36.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	7532	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.59% 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	0.99	6/3707 (0.2%)	1.12	5/5065 (0.1%)
1	B	1.02	5/3644 (0.1%)	1.13	15/4975 (0.3%)
All	All	1.00	11/7351 (0.1%)	1.12	20/10040 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
All	All	0	2

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	244	ALA	C-O	-6.61	1.16	1.24
1	B	246	HIS	C-O	-6.43	1.16	1.24
1	A	476	GLU	C-O	-6.38	1.16	1.24
1	A	243	ALA	C-O	-5.91	1.17	1.24
1	B	244	ALA	C-O	-5.89	1.16	1.23
1	A	475	ALA	CA-CB	-5.70	1.44	1.53
1	B	73	SER	C-O	-5.42	1.17	1.24
1	B	30	VAL	C-O	-5.37	1.18	1.23
1	A	477	VAL	C-O	-5.34	1.18	1.24
1	B	475	ALA	CA-CB	-5.27	1.44	1.53
1	A	453	LEU	C-O	-5.21	1.17	1.23

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	245	ASP	N-CA-C	7.05	119.58	111.11
1	A	42	SER	CA-C-N	6.42	125.99	119.19
1	A	42	SER	C-N-CA	6.42	125.99	119.19
1	B	42	SER	CA-C-N	5.75	125.37	119.56
1	B	42	SER	C-N-CA	5.75	125.37	119.56
1	B	432	ALA	CA-C-N	-5.69	116.28	122.59
1	B	432	ALA	C-N-CA	-5.69	116.28	122.59
1	B	397	ILE	CB-CA-C	-5.57	103.79	111.65
1	A	440	GLY	N-CA-C	-5.56	106.06	112.73
1	B	359	ALA	CA-C-N	-5.51	113.94	122.59
1	B	359	ALA	C-N-CA	-5.51	113.94	122.59
1	B	100	ARG	CA-C-N	-5.50	114.29	119.85
1	B	100	ARG	C-N-CA	-5.50	114.29	119.85
1	A	206	PRO	O-C-N	5.50	123.74	121.15
1	B	245	ASP	N-CA-C	5.38	116.82	111.07
1	B	455	TRP	N-CA-C	-5.31	104.74	111.11
1	B	404	PHE	N-CA-C	5.19	117.43	109.07
1	B	409	GLY	N-CA-C	5.15	119.12	112.83
1	B	477	VAL	CB-CA-C	-5.07	105.48	111.97
1	B	133	GLY	N-CA-C	5.05	119.00	112.54

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	455	TRP	Peptide
1	B	455	TRP	Peptide

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	3624	0	3580	121	0
1	B	3564	0	3516	112	0
2	A	5	0	0	0	0
3	A	170	0	0	6	0
3	B	169	0	0	12	0
All	All	7532	0	7096	233	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 16.

All (233) 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:301:MSE:HE2	1:B:390:HIS:CE1	1.80	1.16
1:B:95:ARG:HD2	1:B:95:ARG:O	1.61	1.01
1:B:261:VAL:HG22	1:B:273:VAL:HG22	1.40	1.00
1:B:458:VAL:HG12	1:B:458:VAL:O	1.59	0.98
1:A:426:ARG:HG3	1:A:426:ARG:HH11	1.30	0.97
1:B:190:LEU:HD21	1:B:286:LEU:HD23	1.44	0.96
1:B:26:LEU:HD21	1:B:446:ALA:HB1	1.51	0.93
1:B:130:THR:HG22	1:B:132:ASN:H	1.32	0.92
1:A:333:GLU:O	1:A:333:GLU:HG3	1.71	0.87
1:B:118:ARG:HD2	3:B:613:HOH:O	1.75	0.85
1:B:301:MSE:CE	1:B:390:HIS:CE1	2.59	0.84
1:A:131:GLY:HA2	1:A:280:SER:HB3	1.58	0.83
1:A:350:GLU:HG2	1:A:351:LYS:N	1.95	0.81
1:B:255:ILE:HG22	1:B:255:ILE:O	1.81	0.81
1:B:301:MSE:HE2	1:B:390:HIS:HE1	1.46	0.80
1:B:458:VAL:O	1:B:458:VAL:CG1	2.30	0.79
1:B:149:HIS:HD2	3:B:633:HOH:O	1.64	0.78
1:A:21:ALA:HB3	1:A:62:VAL:HG13	1.66	0.77
1:B:264:LYS:HE2	3:B:549:HOH:O	1.85	0.77
1:A:289:HIS:HD2	1:A:290:LEU:H	1.32	0.77
1:B:257:ARG:HD2	1:B:403:ARG:NH1	2.00	0.76
1:A:304:THR:HG22	1:A:305:GLY:N	1.99	0.76
1:B:189:ASP:HB2	1:B:196:GLU:HG3	1.69	0.75
1:A:341:LEU:HD21	1:A:366:LEU:HD23	1.73	0.70
1:B:130:THR:HG22	1:B:132:ASN:N	2.06	0.70
1:A:21:ALA:CB	1:A:62:VAL:HG13	2.22	0.69
1:B:179:ARG:HD2	1:B:215:PRO:HA	1.74	0.69
1:B:471:ASP:C	1:B:471:ASP:OD2	2.32	0.69
1:B:110:CYS:HB2	1:B:113:GLU:HG2	1.73	0.69
1:B:179:ARG:HD2	1:B:215:PRO:CA	2.24	0.68
1:B:257:ARG:HD2	1:B:403:ARG:HH12	1.59	0.67
1:B:289:HIS:HD2	1:B:290:LEU:H	1.42	0.67
1:A:275:SER:OG	1:A:399:HIS:HD2	1.78	0.67
1:A:289:HIS:CD2	1:A:290:LEU:H	2.12	0.67
1:B:26:LEU:HD21	1:B:446:ALA:CB	2.22	0.66
1:B:93:ASP:HB3	1:B:99:LEU:HD21	1.77	0.66
1:A:190:LEU:HD21	1:A:286:LEU:HD23	1.77	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:39:THR:O	1:B:50:GLU:HG2	1.96	0.66
1:A:91:LEU:HD11	1:A:146:ILE:HD13	1.75	0.66
1:A:284:LEU:HD13	1:A:394:LEU:HD13	1.78	0.65
1:B:450:GLY:O	1:B:452:ASP:N	2.29	0.65
1:A:350:GLU:HG2	1:A:351:LYS:H	1.60	0.64
1:A:426:ARG:HH11	1:A:426:ARG:CG	2.09	0.64
1:B:110:CYS:H	1:B:136:GLN:NE2	1.95	0.64
1:A:129:ARG:NH2	1:A:198:ASP:OD2	2.30	0.64
1:A:255:ILE:HD13	1:A:262:LEU:HB2	1.78	0.64
1:B:26:LEU:HD23	1:B:453:LEU:CD1	2.28	0.64
1:B:220:LEU:HD12	1:B:220:LEU:O	1.98	0.64
1:A:425:GLN:HE22	1:A:472:PRO:HA	1.63	0.63
1:A:110:CYS:HB2	1:A:113:GLU:HG2	1.79	0.63
1:B:450:GLY:C	1:B:452:ASP:H	2.07	0.62
1:A:281:ASP:C	1:A:283:ARG:H	2.08	0.62
1:A:289:HIS:HD2	1:A:290:LEU:N	1.97	0.61
1:B:333:GLU:O	1:B:333:GLU:HG3	1.99	0.61
1:A:357:PRO:HB2	1:A:497:HIS:CE1	2.37	0.60
1:B:498:ARG:O	1:B:498:ARG:HG2	1.99	0.60
1:A:108:GLY:C	1:A:136:GLN:HE22	2.10	0.60
1:A:426:ARG:HG3	1:A:426:ARG:NH1	2.08	0.60
1:B:289:HIS:CD2	1:B:290:LEU:H	2.17	0.59
1:A:127:LEU:HD23	1:A:132:ASN:C	2.27	0.59
1:A:350:GLU:CG	1:A:351:LYS:N	2.64	0.59
1:A:350:GLU:CG	1:A:351:LYS:H	2.16	0.59
1:B:148:ARG:HG2	1:B:149:HIS:ND1	2.18	0.59
1:A:255:ILE:CD1	1:A:262:LEU:HB2	2.33	0.59
1:B:200:VAL:HG11	1:B:207:PRO:HA	1.85	0.58
1:B:289:HIS:HD2	1:B:290:LEU:N	2.02	0.58
1:A:289:HIS:CD2	1:A:290:LEU:N	2.71	0.58
1:B:100:ARG:HH21	1:B:100:ARG:HG3	1.68	0.58
1:B:218:ARG:HB3	3:B:599:HOH:O	2.03	0.58
1:B:179:ARG:CD	1:B:215:PRO:HA	2.34	0.58
1:B:304:THR:O	1:B:304:THR:HG22	2.04	0.58
1:A:86:LEU:O	1:A:105:GLN:HG2	2.04	0.58
1:A:493:HIS:HB3	1:A:494:PRO:HD3	1.86	0.57
1:B:124:GLU:OE1	1:B:124:GLU:N	2.37	0.57
1:B:8:GLN:HB2	1:B:76:ARG:O	2.04	0.57
1:B:450:GLY:O	1:B:451:ASP:C	2.47	0.57
1:B:454:GLY:N	1:B:457:ASP:OD2	2.24	0.57
1:A:165:ASP:O	1:A:169:MSE:HG3	2.05	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:284:LEU:CD1	1:A:394:LEU:HD13	2.35	0.56
1:A:113:GLU:CD	1:A:113:GLU:H	2.12	0.56
1:A:311:LEU:HG	1:A:315:LEU:HD22	1.86	0.56
1:A:471:ASP:C	1:A:471:ASP:OD1	2.48	0.56
1:A:21:ALA:HB2	1:A:62:VAL:CG1	2.36	0.56
1:A:278:ALA:HB2	1:A:295:TYR:CZ	2.41	0.55
1:A:251:LEU:O	1:A:458:VAL:HG11	2.06	0.55
1:B:301:MSE:CE	1:B:390:HIS:ND1	2.69	0.55
1:A:91:LEU:HD11	1:A:146:ILE:CD1	2.37	0.55
1:B:26:LEU:HD23	1:B:453:LEU:HD12	1.87	0.55
1:A:309:ASN:O	1:A:313:LYS:HG3	2.06	0.55
1:A:189:ASP:HB2	1:A:196:GLU:HG3	1.88	0.55
1:B:108:GLY:C	1:B:136:GLN:HE22	2.15	0.55
1:B:289:HIS:CD2	1:B:290:LEU:N	2.75	0.55
1:A:304:THR:HG22	1:A:305:GLY:H	1.69	0.55
1:B:126:PHE:O	1:B:130:THR:HB	2.08	0.54
1:A:278:ALA:HB2	1:A:295:TYR:CE1	2.43	0.54
1:A:190:LEU:HD21	1:A:286:LEU:CD2	2.38	0.54
1:B:53:ALA:O	1:B:57:ASP:HB2	2.07	0.54
1:A:447:ILE:HD13	1:A:455:TRP:CD2	2.43	0.54
1:B:95:ARG:HD2	1:B:95:ARG:C	2.33	0.54
1:B:91:LEU:HD11	1:B:146:ILE:HD13	1.90	0.54
1:B:321:GLU:HB2	3:B:616:HOH:O	2.07	0.53
1:B:450:GLY:C	1:B:452:ASP:N	2.61	0.53
1:B:19:THR:O	1:B:35:SER:HA	2.09	0.53
1:B:22:ILE:HD12	1:B:24:VAL:CG2	2.40	0.52
1:A:284:LEU:HD12	1:A:397:ILE:HD11	1.91	0.52
1:B:86:LEU:O	1:B:105:GLN:HG2	2.10	0.52
1:B:266:GLY:O	1:B:304:THR:O	2.28	0.52
1:B:124:GLU:N	1:B:124:GLU:CD	2.68	0.52
1:A:281:ASP:OD2	1:A:283:ARG:NE	2.42	0.51
1:A:21:ALA:CB	1:A:62:VAL:CG1	2.87	0.51
1:A:432:ALA:HB3	1:A:463:ARG:HB3	1.92	0.51
1:B:190:LEU:HD21	1:B:286:LEU:CD2	2.30	0.51
1:A:303:ALA:HB1	1:A:307:ALA:HB2	1.93	0.51
1:B:169:MSE:HG2	1:B:174:GLU:O	2.11	0.51
1:B:493:HIS:HB3	1:B:494:PRO:HD3	1.93	0.51
1:B:56:TRP:CD2	1:B:170:LEU:HD23	2.46	0.51
1:A:189:ASP:OD2	1:A:191:ALA:HB3	2.11	0.50
1:A:110:CYS:H	1:A:136:GLN:NE2	2.10	0.50
1:A:281:ASP:O	1:A:283:ARG:N	2.43	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:357:PRO:HB2	1:A:497:HIS:HE1	1.75	0.50
1:B:341:LEU:HD21	1:B:370:HIS:CE1	2.47	0.50
1:B:284:LEU:HD13	1:B:394:LEU:HD13	1.94	0.49
1:A:67:LYS:HG3	1:A:75:TRP:CE2	2.47	0.49
1:A:113:GLU:CD	1:A:113:GLU:N	2.69	0.49
1:A:175:ARG:HD3	3:A:597:HOH:O	2.12	0.49
1:B:284:LEU:CD1	1:B:394:LEU:HD13	2.42	0.49
1:A:447:ILE:HD11	1:A:455:TRP:HA	1.94	0.49
1:B:220:LEU:HD12	1:B:220:LEU:C	2.38	0.49
1:A:220:LEU:HD12	1:A:220:LEU:O	2.13	0.49
1:A:383:VAL:HG11	1:A:416:TRP:HZ2	1.78	0.49
1:A:14:ILE:HG22	1:A:14:ILE:O	2.13	0.49
1:A:124:GLU:OE2	1:A:124:GLU:CA	2.60	0.48
1:A:42:SER:CB	1:A:47:TRP:O	2.61	0.48
1:A:55:TRP:CZ3	1:A:163:SER:HA	2.48	0.48
1:A:139:VAL:HG12	1:A:143:LEU:HD22	1.93	0.48
1:B:456:ASP:OD2	1:B:456:ASP:N	2.42	0.48
1:B:268:ALA:O	1:B:304:THR:OG1	2.29	0.48
1:B:497:HIS:O	1:B:498:ARG:C	2.56	0.48
1:A:257:ARG:CD	3:A:601:HOH:O	2.63	0.47
1:A:273:VAL:HG21	1:A:394:LEU:HG	1.97	0.47
1:B:175:ARG:HD3	3:B:660:HOH:O	2.14	0.47
1:B:321:GLU:CD	3:B:616:HOH:O	2.57	0.47
1:A:425:GLN:NE2	1:A:472:PRO:HA	2.28	0.47
1:B:100:ARG:HG3	1:B:100:ARG:NH2	2.28	0.47
1:B:303:ALA:HB1	1:B:307:ALA:HB2	1.97	0.47
1:A:93:ASP:HB3	1:A:99:LEU:HD21	1.96	0.47
1:A:344:LEU:HD11	1:A:488:LEU:HG	1.96	0.47
1:B:268:ALA:O	1:B:301:MSE:O	2.33	0.47
1:A:281:ASP:CG	1:A:282:PRO:HD2	2.41	0.46
1:A:42:SER:HB3	1:A:47:TRP:O	2.15	0.46
1:A:44:HIS:HB3	1:A:45:PRO:HD2	1.97	0.46
1:B:278:ALA:HB1	1:B:286:LEU:HD21	1.97	0.46
1:B:80:ILE:CG2	1:B:239:VAL:HG22	2.46	0.46
1:A:50:GLU:HG3	1:A:104:GLN:CD	2.40	0.46
1:A:275:SER:OG	1:A:399:HIS:CD2	2.65	0.46
1:A:124:GLU:OE2	1:A:124:GLU:HA	2.16	0.46
1:A:383:VAL:HG11	1:A:416:TRP:CZ2	2.51	0.46
1:B:268:ALA:O	1:B:304:THR:HB	2.16	0.46
1:A:390:HIS:O	1:A:394:LEU:HD22	2.15	0.45
1:B:9:VAL:HG22	1:B:445:ALA:HB3	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:207:PRO:HD2	3:A:582:HOH:O	2.16	0.45
1:A:426:ARG:CG	1:A:426:ARG:NH1	2.72	0.45
1:A:86:LEU:HB2	1:A:87:PRO:HA	1.97	0.45
1:A:459:THR:O	1:A:459:THR:HG23	2.16	0.45
1:B:189:ASP:CB	1:B:196:GLU:HG3	2.44	0.45
1:A:151:PRO:HD2	3:A:642:HOH:O	2.16	0.45
1:A:255:ILE:HG13	1:A:260:ASP:HB3	1.99	0.45
1:B:134:VAL:HA	1:B:138:LEU:HD11	1.98	0.45
1:A:278:ALA:HB2	1:A:295:TYR:CE2	2.52	0.45
1:B:165:ASP:HA	3:B:562:HOH:O	2.17	0.45
1:B:289:HIS:CD2	1:B:291:VAL:H	2.35	0.45
1:A:279:LYS:HD3	1:A:397:ILE:HG22	1.99	0.44
1:A:284:LEU:HD12	1:A:397:ILE:CD1	2.47	0.44
1:A:206:PRO:HA	1:A:207:PRO:HD3	1.84	0.44
1:A:281:ASP:C	1:A:283:ARG:N	2.69	0.44
1:B:268:ALA:O	1:B:304:THR:CB	2.66	0.44
1:B:434:PRO:O	1:B:435:LEU:C	2.60	0.44
1:A:67:LYS:HE3	1:A:75:TRP:NE1	2.32	0.44
1:A:257:ARG:O	1:A:258:PRO:C	2.61	0.44
1:A:291:VAL:HA	1:A:292:PRO:HD3	1.89	0.44
1:A:44:HIS:O	1:A:47:TRP:HB2	2.18	0.43
1:A:105:GLN:H	1:A:105:GLN:NE2	2.16	0.43
1:B:301:MSE:HE1	1:B:390:HIS:ND1	2.32	0.43
1:B:56:TRP:CG	1:B:170:LEU:HD23	2.54	0.43
1:A:91:LEU:CD1	1:A:146:ILE:HD13	2.45	0.43
1:A:174:GLU:HA	1:A:174:GLU:OE1	2.19	0.43
1:A:118:ARG:HG3	1:A:123:SER:OG	2.19	0.43
1:A:315:LEU:C	1:A:317:PRO:HD3	2.43	0.43
1:A:397:ILE:HG22	1:A:397:ILE:O	2.19	0.43
1:B:92:LEU:HA	1:B:97:ALA:O	2.19	0.43
1:B:179:ARG:HD3	3:B:521:HOH:O	2.19	0.43
1:A:257:ARG:HD3	3:A:601:HOH:O	2.17	0.42
1:B:9:VAL:HG22	1:B:445:ALA:CB	2.49	0.42
1:B:162:GLY:HA3	3:B:556:HOH:O	2.18	0.42
1:A:63:LEU:HD13	1:A:233:LEU:HD22	2.01	0.42
1:A:110:CYS:HB2	1:A:113:GLU:CG	2.46	0.42
1:B:458:VAL:CG2	3:B:675:HOH:O	2.66	0.42
1:A:301:MSE:HB2	1:A:301:MSE:HE2	1.76	0.42
1:A:341:LEU:HD23	1:A:341:LEU:HA	1.76	0.42
1:B:380:LEU:HD22	1:B:416:TRP:CG	2.54	0.42
1:A:289:HIS:CD2	1:A:291:VAL:H	2.37	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:271:ILE:HD13	1:A:390:HIS:HB3	2.01	0.42
1:A:346:TYR:O	1:A:360:SER:HA	2.20	0.42
1:A:284:LEU:HD13	1:A:394:LEU:CD1	2.49	0.42
1:B:110:CYS:HB2	1:B:113:GLU:CG	2.48	0.42
1:B:131:GLY:HA2	1:B:280:SER:HB3	2.01	0.42
1:A:348:LEU:O	1:A:358:PHE:CZ	2.72	0.42
1:B:397:ILE:O	1:B:397:ILE:CG2	2.66	0.42
1:A:176:VAL:HG21	1:A:220:LEU:HD13	2.02	0.41
1:A:49:GLU:HA	1:A:102:SER:O	2.19	0.41
1:B:183:LEU:HD23	1:B:287:ASP:HA	2.02	0.41
1:A:143:LEU:HD12	1:A:143:LEU:HA	1.91	0.41
1:B:117:LEU:HD23	1:B:117:LEU:HA	1.93	0.41
1:B:223:VAL:HG21	1:B:233:LEU:HD23	2.02	0.41
1:B:22:ILE:HD12	1:B:24:VAL:HG21	2.03	0.41
1:B:469:THR:HA	1:B:470:PRO:HD3	1.94	0.41
1:A:179:ARG:NH1	3:A:653:HOH:O	2.31	0.41
1:B:86:LEU:CD1	1:B:86:LEU:C	2.94	0.41
1:B:264:LYS:O	1:B:269:GLY:HA2	2.20	0.41
1:A:404:PHE:CE2	1:A:426:ARG:HD3	2.57	0.41
1:B:290:LEU:HD12	1:B:290:LEU:HA	1.88	0.40
1:A:8:GLN:HG3	1:A:76:ARG:NH2	2.36	0.40
1:A:435:LEU:N	1:A:435:LEU:CD1	2.83	0.40
1:B:251:LEU:HD12	1:B:256:THR:HG22	2.03	0.40
1:B:458:VAL:HG22	3:B:675:HOH:O	2.21	0.40
1:B:493:HIS:CE1	1:B:497:HIS:CE1	3.10	0.40
1:A:498:ARG:HH11	1:A:498:ARG:HD2	1.68	0.40
1:B:190:LEU:HD12	1:B:190:LEU:HA	1.74	0.40
1:B:301:MSE:O	1:B:302:ALA:C	2.64	0.40
1:A:67:LYS:HG3	1:A:75:TRP:CD2	2.56	0.40
1:A:278:ALA:HB2	1:A:295:TYR:CD1	2.57	0.40
1:B:11:GLY:O	1:B:21:ALA:HA	2.22	0.40
1:B:184:GLU:OE2	1:B:287:ASP:OD2	2.39	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	484/508 (95%)	463 (96%)	18 (4%)	3 (1%)	21	27
1	B	472/508 (93%)	450 (95%)	18 (4%)	4 (1%)	16	20
All	All	956/1016 (94%)	913 (96%)	36 (4%)	7 (1%)	18	23

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	198	ASP
1	A	456	ASP
1	B	456	ASP
1	B	451	ASP
1	B	450	GLY
1	A	282	PRO
1	B	255	ILE

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	363/374 (97%)	321 (88%)	42 (12%)	5	6
1	B	356/374 (95%)	320 (90%)	36 (10%)	7	9
All	All	719/748 (96%)	641 (89%)	78 (11%)	6	7

All (78) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	VAL
1	A	57	ASP
1	A	62	VAL
1	A	66	LEU
1	A	68	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	72	GLU
1	A	105	GLN
1	A	113	GLU
1	A	118	ARG
1	A	124	GLU
1	A	127	LEU
1	A	137	GLN
1	A	143	LEU
1	A	148	ARG
1	A	170	LEU
1	A	183	LEU
1	A	190	LEU
1	A	202	LEU
1	A	233	LEU
1	A	249	SER
1	A	263	LEU
1	A	272	ILE
1	A	280	SER
1	A	285	TYR
1	A	315	LEU
1	A	318	GLU
1	A	321	GLU
1	A	330	LEU
1	A	333	GLU
1	A	348	LEU
1	A	357	PRO
1	A	375	LEU
1	A	385	LEU
1	A	394	LEU
1	A	425	GLN
1	A	426	ARG
1	A	431	LEU
1	A	451	ASP
1	A	452	ASP
1	A	459	THR
1	A	461	LEU
1	A	498	ARG
1	B	9	VAL
1	B	57	ASP
1	B	66	LEU
1	B	74	ASP
1	B	86	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	95	ARG
1	B	105	GLN
1	B	106	SER
1	B	113	GLU
1	B	116	GLU
1	B	118	ARG
1	B	123	SER
1	B	130	THR
1	B	170	LEU
1	B	190	LEU
1	B	202	LEU
1	B	233	LEU
1	B	255	ILE
1	B	273	VAL
1	B	280	SER
1	B	283	ARG
1	B	290	LEU
1	B	301	MSE
1	B	333	GLU
1	B	348	LEU
1	B	394	LEU
1	B	403	ARG
1	B	412	ARG
1	B	456	ASP
1	B	457	ASP
1	B	458	VAL
1	B	464	THR
1	B	469	THR
1	B	476	GLU
1	B	477	VAL
1	B	498	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	136	GLN
1	A	289	HIS
1	A	390	HIS
1	A	399	HIS
1	A	425	GLN
1	A	493	HIS
1	A	497	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	44	HIS
1	B	58	ASN
1	B	105	GLN
1	B	136	GLN
1	B	137	GLN
1	B	149	HIS
1	B	214	HIS
1	B	289	HIS
1	B	298	ASN
1	B	390	HIS
1	B	425	GLN
1	B	433	ASN
1	B	493	HIS
1	B	497	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](#)

1 ligand is 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	509	-	4,4,4	0.77	0	6,6,6	0.76	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

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

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	483/508 (95%)	0.09	12 (2%) 58 60	15, 25, 40, 54	0
1	B	475/508 (93%)	0.15	17 (3%) 46 48	16, 26, 40, 51	0
All	All	958/1016 (94%)	0.12	29 (3%) 52 54	15, 25, 40, 54	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	358	PHE	5.3
1	B	26	LEU	4.5
1	A	356	ASP	4.0
1	B	453	LEU	3.6
1	A	359	ALA	3.6
1	A	349	GLY	3.5
1	B	458	VAL	3.5
1	A	226	GLU	3.4
1	A	449	GLY	3.4
1	B	280	SER	3.2
1	B	283	ARG	3.1
1	A	463	ARG	3.1
1	A	357	PRO	3.0
1	B	452	ASP	3.0
1	B	476	GLU	2.8
1	A	280	SER	2.8
1	B	25	ARG	2.7
1	B	125	ALA	2.5
1	B	122	ASP	2.5
1	B	348	LEU	2.4
1	B	451	ASP	2.3
1	A	451	ASP	2.3
1	B	302	ALA	2.2
1	B	72	GLU	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	351	LYS	2.1
1	B	358	PHE	2.1
1	B	305	GLY	2.1
1	A	318	GLU	2.1
1	B	464	THR	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
2	PO4	A	509	5/5	0.55	0.28	30,30,30,30	0

6.5 Other polymers [i](#)

There are no such residues in this entry.