Full wwPDB X-ray Structure Validation Report (i)

Oct 19, 2023 – 02:56 AM EDT

PDB ID	:	2OBC
Title	:	The crystal structure of RibD from Escherichia coli in complex with a substrate analogue, ribose 5-phosphate (beta form), bound to the active site of the reductase domain
Authors	:	Moche, M.; Stenmark, P.; Gurmu, D.; Nordlund, P.; Structural Proteomics in Europe (SPINE)
Deposited on	:	2006-12-18
Resolution	:	3.00 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 (i) 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 (i)) were used in the production of this report:

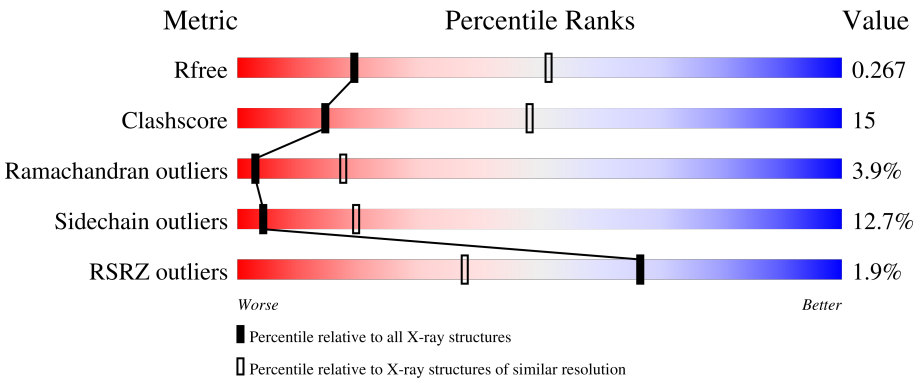
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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 <=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	402	.% 56% 26% 6% 12%
1	B	402	2% 58% 26% 6% 10%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 5534 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 Riboflavin biosynthesis protein ribD.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	354	2719	1711	494	499	6	9	0	0	0
1	B	362	2753	1729	501	511	3	9	0	0	0

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-26	MET	-	cloning artifact	UNP P25539
A	-25	ASP	-	cloning artifact	UNP P25539
A	-24	TYR	-	cloning artifact	UNP P25539
A	-23	LYS	-	cloning artifact	UNP P25539
A	-22	ASP	-	cloning artifact	UNP P25539
A	-21	ASP	-	cloning artifact	UNP P25539
A	-20	ASP	-	cloning artifact	UNP P25539
A	-19	ASP	-	cloning artifact	UNP P25539
A	-18	LYS	-	cloning artifact	UNP P25539
A	-17	GLY	-	cloning artifact	UNP P25539
A	-16	SER	-	cloning artifact	UNP P25539
A	-15	SER	-	cloning artifact	UNP P25539
A	-14	THR	-	cloning artifact	UNP P25539
A	-13	SER	-	cloning artifact	UNP P25539
A	-12	LEU	-	cloning artifact	UNP P25539
A	-11	TYR	-	cloning artifact	UNP P25539
A	-10	LYS	-	cloning artifact	UNP P25539
A	-9	LYS	-	cloning artifact	UNP P25539
A	-8	ALA	-	cloning artifact	UNP P25539
A	-7	GLY	-	cloning artifact	UNP P25539
A	-6	SER	-	cloning artifact	UNP P25539
A	-5	GLU	-	cloning artifact	UNP P25539
A	-4	THR	-	cloning artifact	UNP P25539
A	-3	LEU	-	cloning artifact	UNP P25539
A	-2	TYR	-	cloning artifact	UNP P25539

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	ILE	-	cloning artifact	UNP P25539
A	0	GLN	-	cloning artifact	UNP P25539
A	1	GLY	-	cloning artifact	UNP P25539
A	368	SER	-	expression tag	UNP P25539
A	369	THR	-	expression tag	UNP P25539
A	370	HIS	-	expression tag	UNP P25539
A	371	HIS	-	expression tag	UNP P25539
A	372	HIS	-	expression tag	UNP P25539
A	373	HIS	-	expression tag	UNP P25539
A	374	HIS	-	expression tag	UNP P25539
A	375	HIS	-	expression tag	UNP P25539
B	-26	MET	-	cloning artifact	UNP P25539
B	-25	ASP	-	cloning artifact	UNP P25539
B	-24	TYR	-	cloning artifact	UNP P25539
B	-23	LYS	-	cloning artifact	UNP P25539
B	-22	ASP	-	cloning artifact	UNP P25539
B	-21	ASP	-	cloning artifact	UNP P25539
B	-20	ASP	-	cloning artifact	UNP P25539
B	-19	ASP	-	cloning artifact	UNP P25539
B	-18	LYS	-	cloning artifact	UNP P25539
B	-17	GLY	-	cloning artifact	UNP P25539
B	-16	SER	-	cloning artifact	UNP P25539
B	-15	SER	-	cloning artifact	UNP P25539
B	-14	THR	-	cloning artifact	UNP P25539
B	-13	SER	-	cloning artifact	UNP P25539
B	-12	LEU	-	cloning artifact	UNP P25539
B	-11	TYR	-	cloning artifact	UNP P25539
B	-10	LYS	-	cloning artifact	UNP P25539
B	-9	LYS	-	cloning artifact	UNP P25539
B	-8	ALA	-	cloning artifact	UNP P25539
B	-7	GLY	-	cloning artifact	UNP P25539
B	-6	SER	-	cloning artifact	UNP P25539
B	-5	GLU	-	cloning artifact	UNP P25539
B	-4	THR	-	cloning artifact	UNP P25539
B	-3	LEU	-	cloning artifact	UNP P25539
B	-2	TYR	-	cloning artifact	UNP P25539
B	-1	ILE	-	cloning artifact	UNP P25539
B	0	GLN	-	cloning artifact	UNP P25539
B	1	GLY	-	cloning artifact	UNP P25539
B	368	SER	-	expression tag	UNP P25539
B	369	THR	-	expression tag	UNP P25539
B	370	HIS	-	expression tag	UNP P25539

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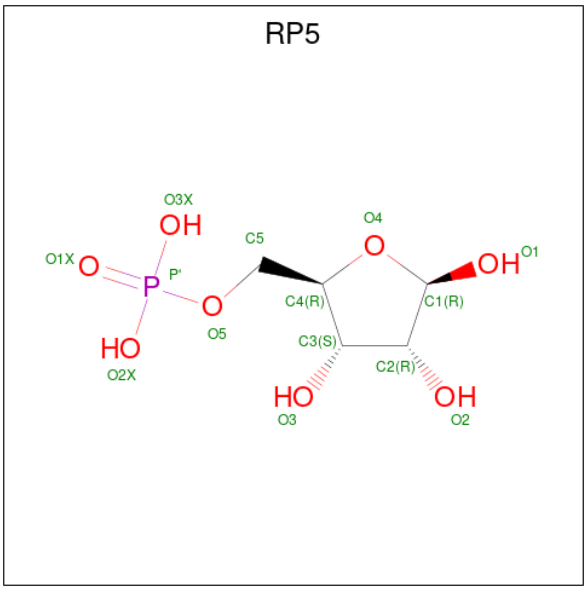
Chain	Residue	Modelled	Actual	Comment	Reference
B	371	HIS	-	expression tag	UNP P25539
B	372	HIS	-	expression tag	UNP P25539
B	373	HIS	-	expression tag	UNP P25539
B	374	HIS	-	expression tag	UNP P25539
B	375	HIS	-	expression tag	UNP P25539

- Molecule 2 is 5-O-phosphono-beta-D-ribofuranose (three-letter code: RP5) (formula: $C_5H_{11}O_8P$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	P		
2	A	1	14	5	8	1	0	0

- Molecule 3 is water.

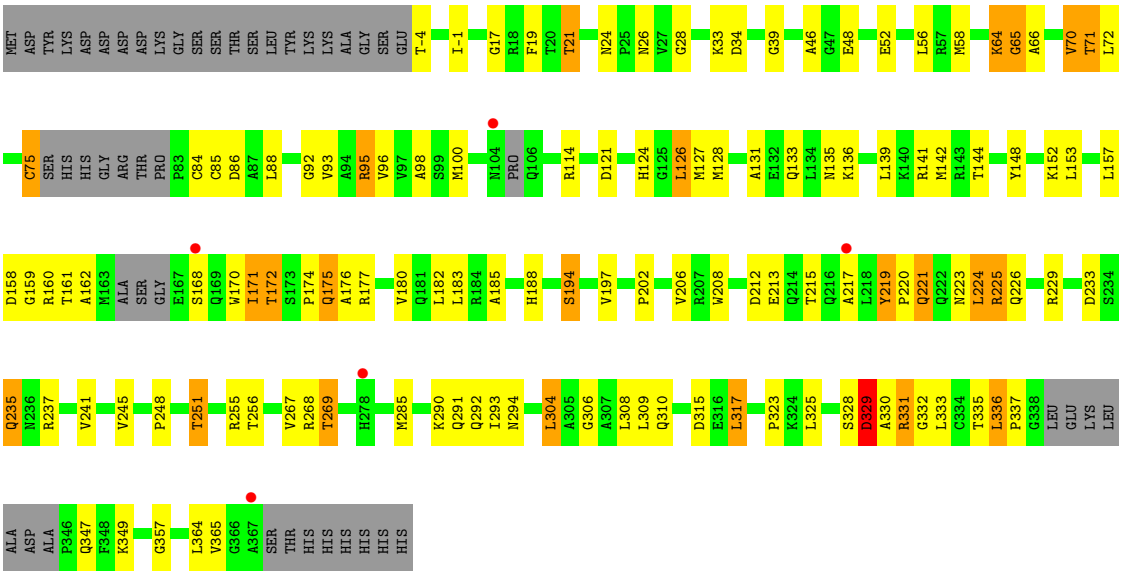
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	31	31	31	0	0
			Total	O		
3	B	17	17	17	0	0

3 Residue-property plots (i)

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

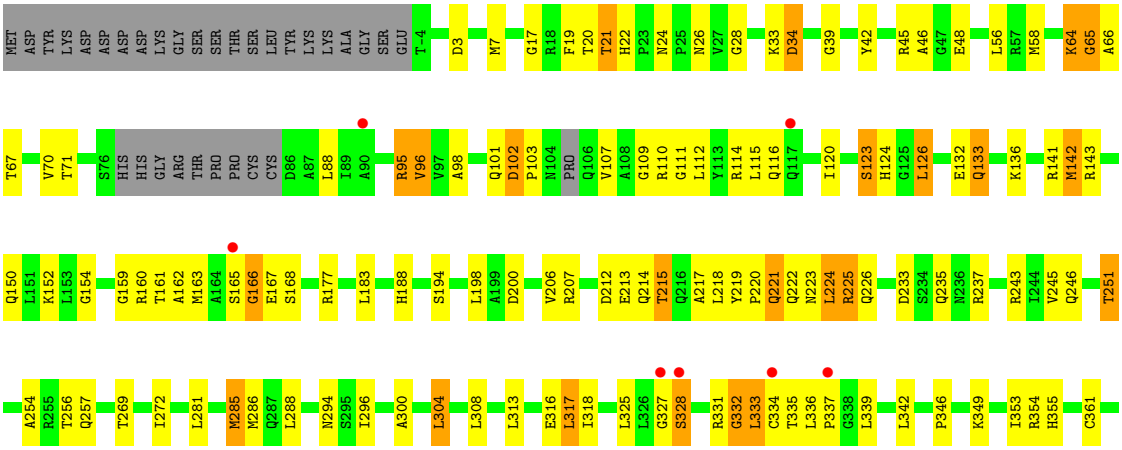
• Molecule 1: Riboflavin biosynthesis protein ribD

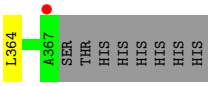
Chain A: %
56% 26% 6% 12%



• Molecule 1: Riboflavin biosynthesis protein ribD

Chain B: 2%
58% 26% 6% 10%




L364
A367
SER
THR
HIS
HIS
HIS
HIS
HIS
HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	173.10Å 173.10Å 76.70Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	28.86 – 3.00 28.85 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.9 (28.86-3.00) 99.9 (28.85-3.00)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	3.22 (at 3.00Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.222 , 0.276 0.214 , 0.267	Depositor DCC
R_{free} test set	1346 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	70.9	Xtriage
Anisotropy	0.006	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 65.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.028 for -h,-k,l	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	5534	wwPDB-VP
Average B, all atoms (Å^2)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.69% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: RP5

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	0.45	0/2761	0.67	1/3729 (0.0%)
1	B	0.45	1/2795 (0.0%)	0.64	0/3781
All	All	0.45	1/5556 (0.0%)	0.65	1/7510 (0.0%)

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	2
1	B	0	2
All	All	0	4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	116	GLN	CD-OE1	5.33	1.35	1.24

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	317	LEU	CA-CB-CG	5.27	127.42	115.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	217	ALA	Peptide

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Mol	Chain	Res	Type	Group
1	A	66	ALA	Peptide
1	B	217	ALA	Peptide
1	B	66	ALA	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	2719	0	2721	87	0
1	B	2753	0	2739	88	0
2	A	14	0	0	0	0
3	A	31	0	0	7	0
3	B	17	0	0	5	0
All	All	5534	0	5460	169	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 (169) 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:194:SER:HB3	1:B:233:ASP:HB3	1.23	1.14
1:B:206:VAL:H	1:B:226:GLN:NE2	1.53	1.06
1:A:75:CYS:HA	1:A:84:CYS:HB3	1.40	1.01
1:B:213:GLU:HA	3:B:390:HOH:O	1.62	0.95
1:A:235:GLN:HG3	1:A:237:ARG:HD2	1.54	0.90
1:B:194:SER:CB	1:B:233:ASP:HB3	2.00	0.90
1:A:39:GLY:HA2	1:A:58:MSE:HE2	1.60	0.83
1:B:206:VAL:H	1:B:226:GLN:HE22	1.26	0.82
1:A:133:GLN:HE21	1:A:136:LYS:HZ2	1.26	0.81
1:B:101:GLN:O	1:B:102:ASP:HB3	1.81	0.78
1:A:309:LEU:HD13	1:B:325:LEU:HD13	1.66	0.76
1:A:206:VAL:H	1:A:226:GLN:NE2	1.83	0.76
1:B:245:VAL:HA	1:B:251:THR:HG21	1.67	0.75
1:A:133:GLN:HE21	1:A:136:LYS:NZ	1.83	0.75
1:A:71:THR:HG22	3:A:421:HOH:O	1.87	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:142:MSE:HA	1:B:142:MSE:HE2	1.71	0.72
1:B:141:ARG:HE	1:B:294:ASN:ND2	1.87	0.72
1:A:175:GLN:HG3	1:A:357:GLY:HA3	1.72	0.72
1:B:42:TYR:OH	1:B:218:LEU:HD22	1.90	0.70
1:A:141:ARG:HE	1:A:294:ASN:ND2	1.88	0.69
1:B:141:ARG:HH11	1:B:294:ASN:HD21	1.40	0.67
1:A:194:SER:HB3	1:A:233:ASP:HB3	1.75	0.67
1:A:160:ARG:HE	1:A:331:ARG:HG2	1.58	0.66
1:A:21:THR:HG23	1:A:24:ASN:O	1.95	0.66
1:B:212:ASP:O	1:B:215:THR:HB	1.96	0.65
1:A:95:ARG:HA	1:A:121:ASP:O	1.96	0.65
1:A:170:TRP:HE3	1:A:177:ARG:HG2	1.62	0.64
1:B:142:MSE:HA	1:B:142:MSE:CE	2.29	0.63
1:B:198:LEU:HD11	1:B:237:ARG:HB3	1.82	0.62
1:B:67:THR:HG23	1:B:95:ARG:HG2	1.81	0.62
1:A:141:ARG:HE	1:A:294:ASN:HD22	1.48	0.61
1:B:160:ARG:HA	1:B:332:GLY:HA3	1.83	0.61
1:A:160:ARG:HE	1:A:331:ARG:CG	2.14	0.61
1:B:141:ARG:HE	1:B:294:ASN:HD22	1.47	0.61
1:A:328:SER:O	1:A:330:ALA:N	2.34	0.60
1:B:101:GLN:O	1:B:102:ASP:CB	2.49	0.60
1:A:33:LYS:CE	1:A:65:GLY:HA3	2.32	0.60
1:A:194:SER:CB	1:A:233:ASP:HB3	2.31	0.60
1:A:158:ASP:HB3	1:B:333:LEU:HD23	1.84	0.60
1:A:33:LYS:HE3	1:A:65:GLY:HA3	1.84	0.59
1:B:110:ARG:CZ	1:B:110:ARG:HA	2.33	0.59
1:B:96:VAL:HG12	1:B:120:ILE:HG21	1.84	0.58
1:A:229:ARG:NH2	1:A:248:PRO:O	2.36	0.58
1:B:188:HIS:CD2	1:B:294:ASN:H	2.22	0.58
1:A:148:TYR:HA	1:A:315:ASP:OD1	2.05	0.56
1:B:33:LYS:HD3	1:B:65:GLY:HA3	1.87	0.56
1:A:162:ALA:HB1	1:A:171:ILE:HG12	1.87	0.56
1:B:3:ASP:HB3	1:B:126:LEU:HD11	1.87	0.56
1:A:188:HIS:CD2	1:A:294:ASN:H	2.23	0.56
1:B:206:VAL:N	1:B:226:GLN:HE22	2.02	0.56
1:B:88:LEU:H	1:B:88:LEU:HD12	1.71	0.54
3:A:404:HOH:O	1:B:355:HIS:HE1	1.91	0.54
1:A:19:PHE:O	1:A:225:ARG:NH1	2.38	0.54
1:B:133:GLN:HE21	1:B:136:LYS:HE3	1.73	0.54
1:A:170:TRP:CE3	1:A:177:ARG:HG2	2.42	0.54
1:A:17:GLY:O	1:A:21:THR:HB	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:24:ASN:ND2	1:B:46:ALA:HA	2.23	0.53
1:A:72:LEU:HD13	1:A:100:MSE:HE3	1.90	0.53
1:B:141:ARG:NH1	1:B:294:ASN:HD21	2.07	0.53
1:A:235:GLN:HG3	1:A:237:ARG:CD	2.34	0.53
1:A:188:HIS:HD2	1:A:294:ASN:H	1.57	0.52
1:A:329:ASP:HA	1:A:331:ARG:HD2	1.91	0.52
1:A:24:ASN:ND2	1:A:46:ALA:HA	2.26	0.51
1:A:245:VAL:HA	1:A:251:THR:HG21	1.92	0.51
1:B:165:SER:O	1:B:166:GLY:C	2.48	0.51
1:A:157:LEU:HD11	1:B:364:LEU:HD22	1.93	0.51
1:B:188:HIS:HD2	1:B:294:ASN:H	1.58	0.50
1:A:141:ARG:HH11	1:A:294:ASN:HD21	1.58	0.50
1:B:98:ALA:O	1:B:124:HIS:HA	2.11	0.50
1:B:353:ILE:O	1:B:353:ILE:HG13	2.11	0.50
1:A:100:MSE:HE2	1:A:131:ALA:HB1	1.93	0.50
1:B:161:THR:O	1:B:163:MSE:N	2.45	0.50
1:A:-4:THR:O	1:A:-1:ILE:N	2.45	0.49
1:A:310:GLN:OE1	1:A:337:PRO:HD2	2.11	0.49
1:B:21:THR:HG21	1:B:26:ASN:OD1	2.12	0.49
1:A:197:VAL:HA	1:A:202:PRO:HD2	1.95	0.48
1:A:161:THR:HG22	1:A:330:ALA:O	2.13	0.48
1:A:306:GLY:HA3	1:A:335:THR:HG22	1.94	0.48
1:B:22:HIS:HB3	1:B:188:HIS:CD2	2.48	0.48
1:A:21:THR:HG21	1:A:26:ASN:OD1	2.14	0.48
1:B:318:ILE:HG23	1:B:361:CYS:SG	2.53	0.48
1:B:233:ASP:HA	3:B:376:HOH:O	2.14	0.48
1:A:317:LEU:HD23	1:A:364:LEU:HB2	1.94	0.48
1:A:176:ALA:O	1:A:180:VAL:HG23	2.13	0.48
1:B:215:THR:OG1	3:B:385:HOH:O	2.10	0.48
1:B:166:GLY:O	1:B:168:SER:N	2.47	0.48
1:B:317:LEU:HD23	1:B:364:LEU:HB2	1.96	0.47
1:B:141:ARG:HH11	1:B:294:ASN:ND2	2.10	0.47
1:B:21:THR:HG23	1:B:24:ASN:O	2.14	0.47
1:A:28:GLY:H	1:A:71:THR:HB	1.79	0.47
1:B:28:GLY:H	1:B:71:THR:HB	1.79	0.47
1:B:154:GLY:O	1:B:161:THR:HG22	2.15	0.47
1:B:300:ALA:HB1	1:B:304:LEU:HB3	1.95	0.47
1:B:7:MSE:HE1	1:B:70:VAL:O	2.13	0.47
1:B:168:SER:HB2	1:B:200:ASP:OD2	2.15	0.46
1:B:206:VAL:H	1:B:226:GLN:HE21	1.54	0.46
1:A:251:THR:HG23	1:A:267:VAL:HG22	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:96:VAL:HG11	1:B:115:LEU:HD13	1.97	0.46
1:A:194:SER:OG	1:A:233:ASP:HB3	2.16	0.46
1:A:136:LYS:HD3	1:A:148:TYR:CZ	2.50	0.46
1:A:328:SER:C	1:A:330:ALA:N	2.69	0.46
1:A:126:LEU:HD22	1:A:127:MSE:HG3	1.99	0.46
1:A:185:ALA:HA	1:A:206:VAL:HG21	1.98	0.45
1:B:19:PHE:O	1:B:225:ARG:HD3	2.16	0.45
1:A:71:THR:CG2	3:A:421:HOH:O	2.54	0.45
1:B:254:ALA:HB1	1:B:272:ILE:HD13	1.98	0.45
1:B:109:GLY:O	1:B:110:ARG:NE	2.50	0.45
1:B:166:GLY:C	1:B:168:SER:H	2.20	0.45
1:B:17:GLY:O	1:B:21:THR:HB	2.16	0.45
1:B:115:LEU:HB3	1:B:120:ILE:HD12	1.99	0.45
1:B:327:GLY:O	1:B:328:SER:C	2.53	0.45
1:A:290:LYS:HE2	3:A:422:HOH:O	2.16	0.45
1:B:39:GLY:HA2	1:B:58:MSE:HE2	1.99	0.45
1:B:281:LEU:HD13	1:B:308:LEU:HD23	1.98	0.45
1:A:325:LEU:HB3	1:B:342:LEU:HD21	1.99	0.45
1:A:141:ARG:O	1:A:144:THR:O	2.34	0.44
1:A:233:ASP:HB2	3:A:420:HOH:O	2.18	0.44
1:A:309:LEU:CD1	1:B:325:LEU:HD13	2.41	0.44
1:B:339:LEU:HD23	1:B:342:LEU:HD22	2.00	0.44
1:B:110:ARG:C	1:B:112:LEU:H	2.21	0.44
1:B:317:LEU:CD2	1:B:364:LEU:HB2	2.47	0.44
1:A:328:SER:C	1:A:330:ALA:H	2.20	0.44
1:B:285:MSE:HG2	1:B:313:LEU:HD13	1.99	0.44
1:A:332:GLY:H	1:B:335:THR:HG22	1.82	0.44
1:A:100:MSE:HE1	1:A:139:LEU:HD11	1.98	0.44
1:A:168:SER:C	1:A:170:TRP:H	2.20	0.44
1:B:212:ASP:OD1	1:B:214:GLN:HG2	2.18	0.44
1:B:220:PRO:HD2	1:B:223:ASN:HD22	1.83	0.44
1:A:304:LEU:HD22	1:A:308:LEU:HG	1.98	0.44
1:A:268:ARG:HH22	1:A:291:GLN:NE2	2.16	0.43
1:B:70:VAL:HG23	1:B:98:ALA:HA	2.00	0.43
1:B:133:GLN:HG3	1:B:136:LYS:NZ	2.33	0.43
1:A:220:PRO:HG2	1:A:223:ASN:ND2	2.33	0.43
1:B:132:GLU:OE2	1:B:143:ARG:NH2	2.51	0.43
1:B:220:PRO:HB2	1:B:222:GLN:HE22	1.82	0.43
1:B:177:ARG:HE	1:B:177:ARG:HB3	1.66	0.43
1:A:52:GLU:OE2	1:A:84:CYS:SG	2.77	0.43
1:A:208:TRP:CZ2	1:A:215:THR:HG23	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:162:ALA:O	1:A:172:THR:HG23	2.19	0.43
1:A:175:GLN:HG3	1:A:357:GLY:CA	2.46	0.43
1:A:335:THR:HG23	1:A:336:LEU:N	2.34	0.43
1:A:219:TYR:CE1	1:A:224:LEU:HA	2.54	0.42
1:B:150:GLN:HA	1:B:316:GLU:O	2.20	0.42
1:B:42:TYR:OH	1:B:218:LEU:CD2	2.65	0.42
1:A:208:TRP:CH2	1:A:215:THR:HG23	2.54	0.42
1:A:188:HIS:HA	1:A:225:ARG:NH2	2.35	0.42
1:B:336:LEU:HA	1:B:337:PRO:HD3	1.81	0.42
1:A:70:VAL:HG23	1:A:98:ALA:HA	2.02	0.42
1:A:269:THR:HG21	3:A:427:HOH:O	2.20	0.42
1:B:288:LEU:HD13	1:B:296:ILE:HD11	2.02	0.41
1:B:218:LEU:HD23	3:B:391:HOH:O	2.20	0.41
1:A:64:LYS:O	1:A:92:GLY:O	2.39	0.41
1:A:160:ARG:NE	1:A:331:ARG:HG2	2.31	0.41
1:A:135:ASN:O	1:A:136:LYS:C	2.58	0.41
1:B:221:GLN:O	1:B:224:LEU:HB2	2.19	0.41
1:A:141:ARG:HG2	1:A:142:MSE:HE2	2.02	0.41
1:A:323:PRO:HG3	3:A:410:HOH:O	2.20	0.41
1:A:133:GLN:HG3	1:A:136:LYS:HZ2	1.85	0.41
1:A:161:THR:HG23	1:A:161:THR:O	2.20	0.41
1:B:286:MSE:HE2	1:B:286:MSE:HB3	1.79	0.41
1:B:45:ARG:NH2	1:B:45:ARG:HB2	2.36	0.40
1:B:141:ARG:NE	1:B:294:ASN:ND2	2.63	0.40
1:A:335:THR:HG23	1:A:336:LEU:H	1.86	0.40
1:A:158:ASP:OD1	1:A:158:ASP:N	2.52	0.40
1:B:355:HIS:HD2	3:B:377:HOH:O	2.04	0.40
1:A:98:ALA:O	1:A:124:HIS:HA	2.21	0.40
1:B:159:GLY:HA3	1:B:334:CYS:CB	2.50	0.40
1:A:291:GLN:O	1:A:292:GLN:HB2	2.21	0.40
1:B:243:ARG:O	1:B:246:GLN:HG2	2.22	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	344/402 (86%)	308 (90%)	26 (8%)	10 (3%)	4	24
1	B	356/402 (89%)	310 (87%)	29 (8%)	17 (5%)	2	13
All	All	700/804 (87%)	618 (88%)	55 (8%)	27 (4%)	3	17

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	172	THR
1	A	329	ASP
1	B	107	VAL
1	B	162	ALA
1	B	167	GLU
1	B	221	GLN
1	B	328	SER
1	A	34	ASP
1	A	95	ARG
1	A	333	LEU
1	B	34	ASP
1	B	65	GLY
1	B	102	ASP
1	B	166	GLY
1	B	331	ARG
1	B	346	PRO
1	A	174	PRO
1	A	159	GLY
1	A	212	ASP
1	B	95	ARG
1	A	221	GLN
1	B	64	LYS
1	B	103	PRO
1	B	111	GLY
1	B	123	SER
1	B	332	GLY
1	A	65	GLY

5.3.2 Protein sidechains (i)

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	284/321 (88%)	242 (85%)	42 (15%)	3 14
1	B	283/321 (88%)	253 (89%)	30 (11%)	6 26
All	All	567/642 (88%)	495 (87%)	72 (13%)	4 19

All (72) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	THR
1	A	48	GLU
1	A	56	LEU
1	A	64	LYS
1	A	70	VAL
1	A	71	THR
1	A	75	CYS
1	A	85	CYS
1	A	86	ASP
1	A	88	LEU
1	A	93	VAL
1	A	96	VAL
1	A	114	ARG
1	A	126	LEU
1	A	128	MSE
1	A	152	LYS
1	A	153	LEU
1	A	171	ILE
1	A	175	GLN
1	A	182	LEU
1	A	183	LEU
1	A	194	SER
1	A	213	GLU
1	A	219	TYR
1	A	221	GLN
1	A	224	LEU
1	A	225	ARG
1	A	235	GLN
1	A	241	VAL
1	A	251	THR
1	A	255	ARG

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Mol	Chain	Res	Type
1	A	256	THR
1	A	269	THR
1	A	285	MSE
1	A	293	ILE
1	A	304	LEU
1	A	329	ASP
1	A	331	ARG
1	A	336	LEU
1	A	347	GLN
1	A	349	LYS
1	A	365	VAL
1	B	20	THR
1	B	21	THR
1	B	34	ASP
1	B	48	GLU
1	B	56	LEU
1	B	64	LYS
1	B	96	VAL
1	B	114	ARG
1	B	123	SER
1	B	126	LEU
1	B	133	GLN
1	B	142	MSE
1	B	152	LYS
1	B	183	LEU
1	B	207	ARG
1	B	215	THR
1	B	219	TYR
1	B	224	LEU
1	B	225	ARG
1	B	235	GLN
1	B	251	THR
1	B	256	THR
1	B	257	GLN
1	B	269	THR
1	B	285	MSE
1	B	304	LEU
1	B	317	LEU
1	B	333	LEU
1	B	349	LYS
1	B	354	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	133	GLN
1	A	150	GLN
1	A	188	HIS
1	A	222	GLN
1	A	226	GLN
1	A	235	GLN
1	A	246	GLN
1	A	291	GLN
1	A	292	GLN
1	A	294	ASN
1	B	133	GLN
1	B	188	HIS
1	B	222	GLN
1	B	223	ASN
1	B	226	GLN
1	B	235	GLN
1	B	246	GLN
1	B	291	GLN
1	B	294	ASN

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 monosaccharides 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	RP5	A	401	-	14,14,14	0.59	0	20,21,21	1.33	5 (25%)

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
2	RP5	A	401	-	-	4/6/22/22	0/1/1/1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	401	RP5	O4-C1-C2	2.77	107.88	104.46
2	A	401	RP5	O1-C1-O4	-2.37	108.10	111.13
2	A	401	RP5	C2-C3-C4	2.13	106.79	102.64
2	A	401	RP5	O3X-P'-O2X	2.04	115.42	107.64
2	A	401	RP5	C1-C2-C3	2.04	104.85	102.30

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	RP5	C5-O5-P'-O1X
2	A	401	RP5	C5-O5-P'-O2X
2	A	401	RP5	C5-O5-P'-O3X
2	A	401	RP5	O4-C4-C5-O5

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)

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	345/402 (85%)	-0.23	5 (1%)	75	49	43, 56, 75, 94	0
1	B	353/402 (87%)	-0.17	8 (2%)	60	31	44, 58, 73, 80	0
All	All	698/804 (86%)	-0.20	13 (1%)	66	37	43, 58, 75, 94	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	334	CYS	3.9
1	B	337	PRO	3.5
1	B	328	SER	2.8
1	A	278	HIS	2.4
1	B	327	GLY	2.4
1	A	168	SER	2.3
1	B	90	ALA	2.3
1	B	165	SER	2.3
1	A	217	ALA	2.3
1	B	117	GLN	2.1
1	B	367	ALA	2.1
1	A	104	ASN	2.1
1	A	367	ALA	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 monosaccharides 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(Å^2)	Q<0.9
2	RP5	A	401	14/14	0.91	0.19	75,81,82,82	0

6.5 Other polymers (i)

There are no such residues in this entry.