



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 12:39 AM UTC

PDB ID : 3B4T / pdb_00003b4t
Title : Crystal structure of Mycobacterium tuberculosis RNase PH, the Mycobacterium tuberculosis Structural Genomics Consortium target Rv1340
Authors : Antczak, A.J.; Berger, J.M.; Lakin, T.; Segelke, B.W.; Mycobacterium Tuberculosis Structural Proteomics Project (XMTB); TB Structural Genomics Consortium (TBSGC)
Deposited on : 2007-10-24
Resolution : 2.10 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

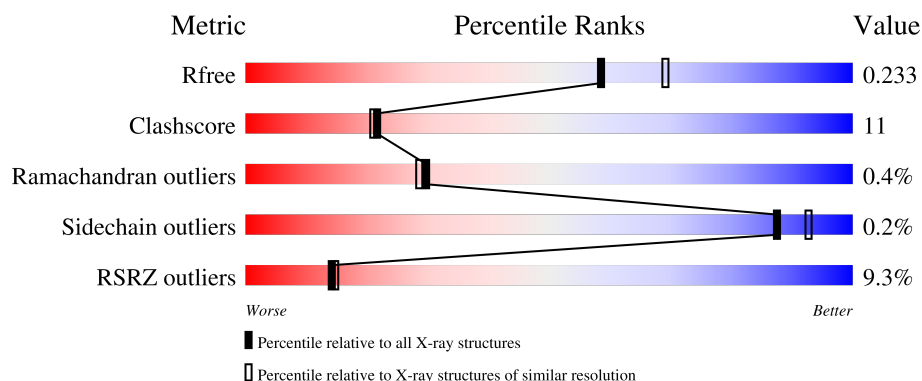
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	262	7% 75% 17% 7%
1	B	262	8% 74% 17% 9%
1	C	262	6% 77% 14% • 8%
1	D	262	10% 73% 18% • 9%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	E	262	11% 76% 15% 8%
1	F	262	8% 75% 16% 8%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 11806 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 Ribonuclease PH.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	243	Total	C	N	O	S	0	0	0
			1787	1105	318	356	8			
1	B	239	Total	C	N	O	S	0	0	0
			1765	1093	314	350	8			
1	C	241	Total	C	N	O	S	0	0	0
			1790	1110	320	352	8			
1	D	239	Total	C	N	O	S	0	0	0
			1765	1093	314	350	8			
1	E	240	Total	C	N	O	S	0	0	0
			1771	1096	315	352	8			
1	F	240	Total	C	N	O	S	0	0	0
			1771	1096	315	352	8			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLY	-	expression tag	UNP Q10628
A	-2	SER	-	expression tag	UNP Q10628
A	-1	HIS	-	expression tag	UNP Q10628
A	0	VAL	-	expression tag	UNP Q10628
B	-3	GLY	-	expression tag	UNP Q10628
B	-2	SER	-	expression tag	UNP Q10628
B	-1	HIS	-	expression tag	UNP Q10628
B	0	VAL	-	expression tag	UNP Q10628
C	-3	GLY	-	expression tag	UNP Q10628
C	-2	SER	-	expression tag	UNP Q10628
C	-1	HIS	-	expression tag	UNP Q10628
C	0	VAL	-	expression tag	UNP Q10628
D	-3	GLY	-	expression tag	UNP Q10628
D	-2	SER	-	expression tag	UNP Q10628
D	-1	HIS	-	expression tag	UNP Q10628
D	0	VAL	-	expression tag	UNP Q10628
E	-3	GLY	-	expression tag	UNP Q10628

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
E	-2	SER	-	expression tag	UNP Q10628
E	-1	HIS	-	expression tag	UNP Q10628
E	0	VAL	-	expression tag	UNP Q10628
F	-3	GLY	-	expression tag	UNP Q10628
F	-2	SER	-	expression tag	UNP Q10628
F	-1	HIS	-	expression tag	UNP Q10628
F	0	VAL	-	expression tag	UNP Q10628

- Molecule 2 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



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		
2	C	1	Total	O	P	0	0
			5	4	1		
2	C	1	Total	O	P	0	0
			5	4	1		
2	D	1	Total	O	P	0	0
			5	4	1		
2	D	1	Total	O	P	0	0
			5	4	1		
2	E	1	Total	O	P	0	0
			5	4	1		

Continued on next page...

Continued from previous page...

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

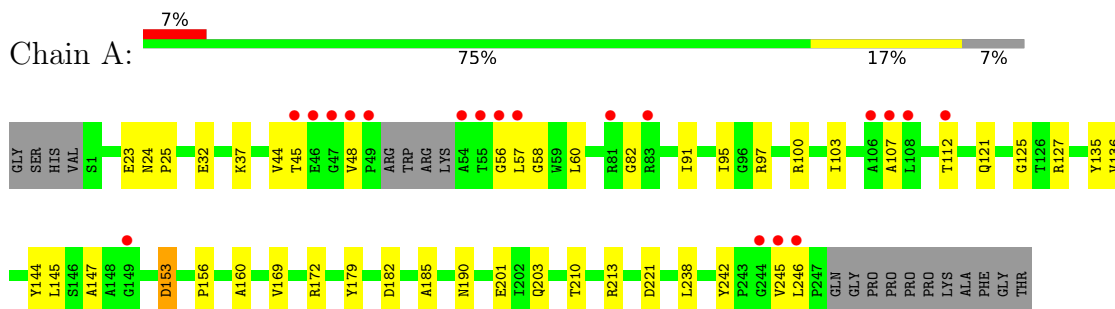
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	214	Total	O	0	0
			214	214		
3	B	184	Total	O	0	0
			184	184		
3	C	192	Total	O	0	0
			192	192		
3	D	173	Total	O	0	0
			173	173		
3	E	185	Total	O	0	0
			185	185		
3	F	159	Total	O	0	0
			159	159		

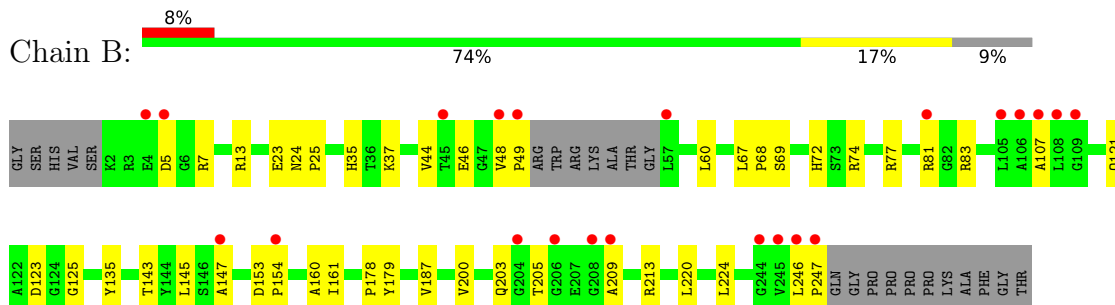
3 Residue-property plots

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.

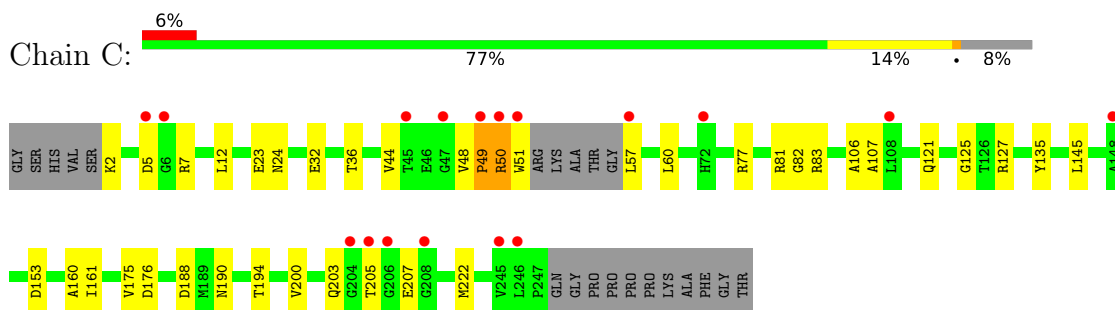
• Molecule 1: Ribonuclease PH



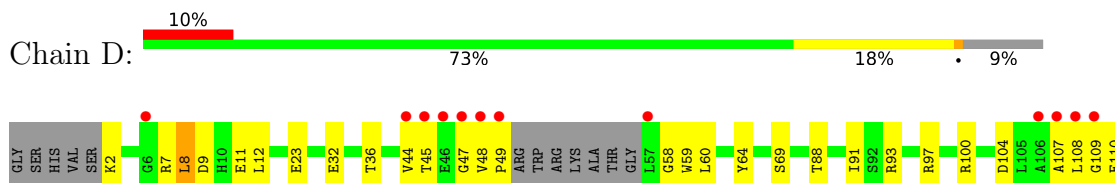
• Molecule 1: Ribonuclease PH



• Molecule 1: Ribonuclease PH

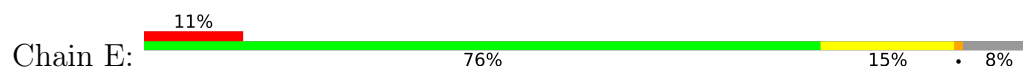


• Molecule 1: Ribonuclease PH

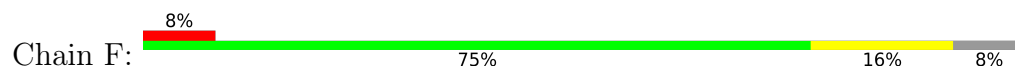




● Molecule 1: Ribonuclease PH



● Molecule 1: Ribonuclease PH



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	73.53Å 152.41Å 83.51Å 90.00° 109.46° 90.00°	Depositor
Resolution (Å)	39.69 – 2.10 39.69 – 2.10	Depositor EDS
% Data completeness (in resolution range)	91.4 (39.69-2.10) 99.7 (39.69-2.10)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.67 (at 2.08Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.194 , 0.229 0.203 , 0.233	Depositor DCC
R_{free} test set	5089 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	32.3	Xtriage
Anisotropy	0.363	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 47.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	11806	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.66% 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	0.31	0/1809	0.71	4/2459 (0.2%)
1	B	0.31	0/1787	0.72	0/2429
1	C	0.34	1/1814 (0.1%)	0.74	0/2466
1	D	0.29	0/1787	0.70	0/2429
1	E	0.30	0/1793	0.72	1/2437 (0.0%)
1	F	0.28	0/1793	0.70	0/2437
All	All	0.31	1/10783 (0.0%)	0.71	5/14657 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	50	ARG	C-O	-6.31	1.16	1.24

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	45	THR	N-CA-C	5.35	117.11	109.14
1	A	153	ASP	CA-C-N	5.21	124.87	119.56
1	A	153	ASP	C-N-CA	5.21	124.87	119.56
1	A	242	TYR	CA-C-N	5.15	124.87	119.82
1	A	242	TYR	C-N-CA	5.15	124.87	119.82

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	1787	0	1794	43	0
1	B	1765	0	1771	44	0
1	C	1790	0	1794	49	0
1	D	1765	0	1771	49	0
1	E	1771	0	1779	32	0
1	F	1771	0	1779	33	0
2	A	10	0	0	0	0
2	B	5	0	0	0	0
2	C	10	0	0	0	0
2	D	10	0	0	1	0
2	E	5	0	0	0	0
2	F	10	0	0	0	0
3	A	214	0	0	13	0
3	B	184	0	0	10	0
3	C	192	0	0	11	0
3	D	173	0	0	7	0
3	E	185	0	0	2	0
3	F	159	0	0	9	0
All	All	11806	0	10688	231	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 11.

All (231) 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:E:244:GLY:HA2	1:E:245:VAL:HB	1.59	0.85
1:A:44:VAL:HG11	1:A:145:LEU:HD21	1.60	0.83
1:A:127:ARG:HD2	1:A:203:GLN:HE22	1.43	0.83
1:C:107:ALA:HB1	1:C:153:ASP:HB3	1.59	0.82
1:F:107:ALA:HB1	1:F:153:ASP:HB3	1.61	0.82
1:D:127:ARG:HD2	2:D:260:PO4:O2	1.81	0.79
1:C:175:VAL:HG13	1:C:222:MET:HG3	1.64	0.78
1:C:48:VAL:CG1	1:C:49:PRO:HD2	2.15	0.77
1:C:48:VAL:HG13	1:C:49:PRO:HD2	1.67	0.75
1:D:107:ALA:HB1	1:D:153:ASP:HB2	1.68	0.74
1:C:48:VAL:HG11	1:C:51:TRP:HB2	1.69	0.73
1:C:23:GLU:HG3	3:C:392:HOH:O	1.89	0.73
1:D:45:THR:CG2	1:D:112:THR:HB	2.19	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:107:ALA:HB1	1:A:153:ASP:HB2	1.70	0.72
1:D:127:ARG:HD3	1:D:190:ASN:ND2	2.05	0.72
1:E:107:ALA:HB1	1:E:153:ASP:HB3	1.73	0.71
1:A:91:ILE:HG13	3:A:317:HOH:O	1.90	0.69
1:B:107:ALA:HB1	1:B:153:ASP:HB3	1.74	0.69
1:B:25:PRO:HG3	1:F:69:SER:HB2	1.77	0.67
1:B:187:VAL:HG22	1:B:209:ALA:HB1	1.78	0.66
1:B:187:VAL:HG21	3:B:429:HOH:O	1.95	0.66
1:C:127:ARG:NH1	1:C:203:GLN:HE22	1.94	0.66
1:C:48:VAL:CG1	1:C:51:TRP:HB2	2.27	0.65
1:B:48:VAL:HG12	1:B:49:PRO:HD2	1.79	0.65
3:E:461:HOH:O	1:F:89:GLN:HG3	1.97	0.65
1:C:51:TRP:O	1:C:51:TRP:CD1	2.50	0.64
1:A:121:GLN:HE22	1:C:23:GLU:HB2	1.63	0.64
1:B:69:SER:HB2	1:F:25:PRO:HG3	1.78	0.64
1:C:127:ARG:HH11	1:C:203:GLN:HE22	1.47	0.63
1:C:205:THR:HB	3:D:444:HOH:O	1.97	0.63
1:B:44:VAL:HG11	1:B:145:LEU:HD21	1.81	0.63
1:A:23:GLU:H	1:C:121:GLN:HE22	1.46	0.62
1:F:44:VAL:HG11	1:F:145:LEU:HD21	1.82	0.62
1:C:175:VAL:HG13	1:C:222:MET:CG	2.31	0.61
3:A:406:HOH:O	1:B:203:GLN:HA	2.00	0.61
1:C:44:VAL:HG11	1:C:145:LEU:HD21	1.83	0.61
1:C:175:VAL:CG1	1:C:222:MET:HG3	2.31	0.61
1:B:48:VAL:CG1	1:B:49:PRO:HD2	2.31	0.60
1:B:5:ASP:OD2	1:B:7:ARG:NE	2.26	0.60
1:A:82:GLY:HA2	3:A:457:HOH:O	2.01	0.60
1:E:127:ARG:HD2	1:E:190:ASN:ND2	2.17	0.60
1:C:48:VAL:HG11	1:C:51:TRP:CB	2.32	0.60
1:C:5:ASP:HB2	3:C:393:HOH:O	2.02	0.59
1:C:51:TRP:CZ2	1:C:57:LEU:HB2	2.37	0.59
1:D:11:GLU:HG2	3:D:391:HOH:O	2.01	0.59
1:D:108:LEU:HD12	1:D:151:LEU:HD21	1.83	0.59
1:E:245:VAL:HG12	1:E:245:VAL:O	2.03	0.59
1:A:45:THR:HB	1:A:112:THR:CG2	2.33	0.58
1:A:32:GLU:HG2	1:A:37:LYS:HG2	1.86	0.58
1:D:91:ILE:HG13	3:D:325:HOH:O	2.04	0.57
1:F:182:ASP:HB3	3:F:374:HOH:O	2.04	0.57
1:A:127:ARG:HD2	1:A:203:GLN:NE2	2.16	0.57
1:A:179:TYR:HA	3:A:452:HOH:O	2.03	0.57
1:A:182:ASP:HB3	3:A:452:HOH:O	2.04	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:45:THR:HG22	1:D:112:THR:HB	1.85	0.57
1:F:104:ASP:HB3	1:F:107:ALA:HB3	1.87	0.57
1:E:12:LEU:HD21	1:E:226:ALA:HB1	1.87	0.56
1:D:7:ARG:HH22	1:D:178:PRO:HD3	1.69	0.56
1:D:44:VAL:HG12	1:D:45:THR:N	2.20	0.56
1:E:244:GLY:HA2	1:E:245:VAL:CB	2.34	0.56
1:B:81:ARG:HH12	1:B:83:ARG:HH21	1.53	0.56
1:A:221:ASP:OD1	1:B:213:ARG:NH1	2.38	0.56
1:A:100:ARG:HA	1:A:103:ILE:HG22	1.88	0.56
1:D:146:SER:HB3	1:D:151:LEU:HD12	1.88	0.56
1:C:57:LEU:HD22	1:C:106:ALA:HB2	1.88	0.55
1:F:188:ASP:O	1:F:205:THR:HA	2.05	0.55
1:C:200:VAL:HG22	1:D:210:THR:HG22	1.88	0.55
1:D:47:GLY:HA2	1:D:110:GLU:O	2.05	0.55
1:D:127:ARG:HD3	1:D:190:ASN:HD21	1.69	0.55
1:E:1:SER:H2	1:E:172:ARG:HH12	1.54	0.55
1:A:23:GLU:H	1:C:121:GLN:NE2	2.04	0.55
3:C:453:HOH:O	1:D:97:ARG:NH1	2.40	0.55
1:A:121:GLN:NE2	1:C:23:GLU:H	2.05	0.54
1:B:81:ARG:NH1	1:B:83:ARG:HH21	2.05	0.54
1:A:213:ARG:NH2	3:A:453:HOH:O	2.40	0.54
1:B:46:GLU:HA	3:B:422:HOH:O	2.08	0.54
1:F:12:LEU:HD21	1:F:226:ALA:HB1	1.89	0.54
1:B:121:GLN:HE22	1:F:23:GLU:CD	2.16	0.54
1:B:153:ASP:CG	1:B:154:PRO:HD2	2.33	0.54
1:D:48:VAL:HA	1:D:112:THR:OG1	2.07	0.54
1:A:45:THR:HB	1:A:112:THR:HG23	1.89	0.54
1:C:83:ARG:HD2	3:E:508:HOH:O	2.08	0.53
1:D:135:TYR:CE1	1:D:160:ALA:HA	2.43	0.53
1:A:172:ARG:HD2	3:A:445:HOH:O	2.07	0.53
1:C:51:TRP:CH2	1:C:57:LEU:HD12	2.43	0.53
1:B:205:THR:HB	3:B:406:HOH:O	2.09	0.53
1:D:8:LEU:C	3:D:391:HOH:O	2.51	0.53
1:D:9:ASP:OD2	1:D:172:ARG:HD3	2.09	0.53
1:D:135:TYR:CZ	1:D:160:ALA:HA	2.43	0.53
1:A:135:TYR:CZ	1:A:160:ALA:HA	2.44	0.53
1:D:69:SER:HB2	1:E:25:PRO:HG3	1.91	0.53
1:D:45:THR:HG21	3:D:403:HOH:O	2.08	0.52
1:D:12:LEU:HD11	1:D:226:ALA:HB1	1.91	0.52
1:E:1:SER:N	1:E:172:ARG:HH12	2.07	0.52
1:A:147:ALA:CB	1:A:246:LEU:HB3	2.39	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:51:TRP:O	1:C:51:TRP:CG	2.59	0.52
1:C:50:ARG:O	1:C:51:TRP:C	2.53	0.52
1:E:44:VAL:HG11	1:E:145:LEU:HD21	1.92	0.52
1:A:24:ASN:HB2	3:C:380:HOH:O	2.09	0.52
1:C:135:TYR:CZ	1:C:160:ALA:HA	2.45	0.52
1:D:201:GLU:HB2	3:D:436:HOH:O	2.09	0.51
1:E:200:VAL:HG22	1:F:210:THR:HG22	1.93	0.51
1:E:135:TYR:CZ	1:E:160:ALA:HA	2.45	0.51
1:B:246:LEU:HD22	3:B:421:HOH:O	2.10	0.50
1:E:109:GLY:O	1:E:110:GLU:C	2.54	0.50
1:C:48:VAL:CG1	1:C:49:PRO:CD	2.87	0.50
1:E:244:GLY:CA	1:E:245:VAL:HB	2.37	0.50
1:F:57:LEU:HD22	1:F:106:ALA:HB2	1.93	0.50
1:D:7:ARG:NH2	1:D:178:PRO:HD3	2.27	0.49
1:F:60:LEU:HD13	1:F:103:ILE:CD1	2.42	0.49
1:D:45:THR:HG21	1:D:112:THR:HB	1.93	0.49
1:C:2:LYS:HB3	3:C:438:HOH:O	2.13	0.49
1:D:48:VAL:HB	1:D:49:PRO:CD	2.43	0.49
3:A:453:HOH:O	1:B:220:LEU:HB3	2.13	0.48
1:F:188:ASP:O	1:F:189:MET:HB3	2.11	0.48
1:A:136:VAL:HG13	1:A:238:LEU:HD21	1.95	0.48
1:A:210:THR:HG22	1:B:200:VAL:HG22	1.95	0.48
1:C:48:VAL:CG1	1:C:51:TRP:CB	2.92	0.48
1:F:81:ARG:HH12	1:F:83:ARG:NH2	2.11	0.48
1:B:74:ARG:NH2	3:F:416:HOH:O	2.47	0.48
1:E:103:ILE:HD11	1:E:138:LEU:HD21	1.94	0.48
1:C:60:LEU:C	1:C:60:LEU:HD23	2.38	0.48
1:B:72:HIS:HE1	1:B:179:TYR:CD2	2.32	0.47
1:C:51:TRP:CZ2	1:C:57:LEU:HD12	2.49	0.47
3:A:324:HOH:O	1:C:24:ASN:HB2	2.13	0.47
1:A:100:ARG:HA	1:A:103:ILE:CG2	2.44	0.47
1:B:135:TYR:CZ	1:B:160:ALA:HA	2.49	0.47
1:B:68:PRO:HG2	3:F:416:HOH:O	2.15	0.47
1:E:242:TYR:CE2	1:E:244:GLY:HA3	2.50	0.47
1:E:66:MET:HE2	1:E:66:MET:HB3	1.81	0.46
1:B:35:HIS:ND1	1:F:23:GLU:OE2	2.49	0.46
1:F:66:MET:HE3	1:F:122:ALA:HB2	1.96	0.46
1:D:201:GLU:HG3	1:D:202:ILE:N	2.30	0.46
1:E:107:ALA:CB	1:E:153:ASP:HB3	2.42	0.46
1:C:48:VAL:HG12	1:C:49:PRO:HD2	1.93	0.45
1:E:60:LEU:C	1:E:60:LEU:HD23	2.41	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:77:ARG:NE	3:F:416:HOH:O	2.48	0.45
1:F:127:ARG:HD2	1:F:190:ASN:ND2	2.32	0.45
1:A:48:VAL:HG21	1:A:58:GLY:HA2	1.97	0.45
1:F:71:THR:HA	3:F:404:HOH:O	2.16	0.45
1:A:125:GLY:HA2	3:A:277:HOH:O	2.16	0.45
1:B:123:ASP:O	1:B:178:PRO:HA	2.17	0.45
1:B:77:ARG:HD3	3:B:304:HOH:O	2.15	0.45
1:D:44:VAL:CG1	1:D:45:THR:N	2.79	0.45
1:D:12:LEU:HD12	1:D:12:LEU:N	2.31	0.45
1:E:173:ILE:HG23	1:E:219:LEU:HD23	1.99	0.45
1:F:206:GLY:HA3	3:F:387:HOH:O	2.16	0.45
1:C:7:ARG:HH12	1:C:176:ASP:HB3	1.82	0.44
1:C:190:ASN:HD22	1:C:203:GLN:HE21	1.62	0.44
1:D:59:TRP:O	1:D:112:THR:HA	2.17	0.44
1:A:60:LEU:C	1:A:60:LEU:HD23	2.42	0.44
1:D:2:LYS:HB3	3:D:450:HOH:O	2.17	0.44
1:F:122:ALA:HB3	3:F:404:HOH:O	2.17	0.44
1:D:47:GLY:O	1:D:112:THR:OG1	2.31	0.44
1:D:60:LEU:HD23	1:D:60:LEU:C	2.42	0.44
1:A:245:VAL:HG23	1:A:245:VAL:O	2.17	0.44
3:B:351:HOH:O	1:F:72:HIS:HE1	2.00	0.44
1:E:242:TYR:HA	1:E:243:PRO:HD3	1.86	0.44
1:B:143:THR:HG22	3:B:421:HOH:O	2.17	0.44
1:D:12:LEU:HD11	1:D:226:ALA:CB	2.47	0.44
1:B:161:ILE:CD1	1:B:200:VAL:HG21	2.48	0.44
1:F:135:TYR:CZ	1:F:160:ALA:HA	2.52	0.44
1:B:37:LYS:HE2	3:F:379:HOH:O	2.18	0.43
1:C:81:ARG:HD2	3:C:391:HOH:O	2.18	0.43
1:D:23:GLU:HB2	1:E:121:GLN:HE22	1.82	0.43
1:D:104:ASP:HB3	1:D:107:ALA:HB3	2.00	0.43
1:C:127:ARG:HH11	1:C:203:GLN:NE2	2.15	0.43
1:F:246:LEU:HD12	1:F:247:PRO:HD2	2.00	0.43
1:A:56:GLY:C	1:A:57:LEU:HD12	2.42	0.43
1:E:108:LEU:HD12	1:E:151:LEU:HD23	2.00	0.43
1:B:7:ARG:CZ	1:B:13:ARG:HG3	2.48	0.43
1:E:201:GLU:HG3	1:E:202:ILE:N	2.33	0.43
1:A:121:GLN:HE22	1:C:23:GLU:H	1.66	0.43
1:B:153:ASP:OD1	1:B:154:PRO:HD2	2.18	0.43
1:C:82:GLY:HA2	3:C:398:HOH:O	2.19	0.43
1:D:64:TYR:O	1:D:88:THR:HG23	2.18	0.43
1:A:44:VAL:CG1	1:A:145:LEU:HD21	2.41	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:453:HOH:O	1:D:93:ARG:HB3	2.18	0.43
1:C:125:GLY:HA2	3:C:274:HOH:O	2.19	0.43
1:D:32:GLU:HA	1:D:36:THR:O	2.19	0.42
1:B:60:LEU:HD23	1:B:60:LEU:C	2.44	0.42
1:D:23:GLU:H	1:E:121:GLN:NE2	2.17	0.42
1:A:144:TYR:HA	1:A:246:LEU:HD22	2.01	0.42
1:F:57:LEU:HD22	1:F:106:ALA:CB	2.49	0.42
1:F:109:GLY:C	1:F:111:ASN:H	2.26	0.42
1:D:109:GLY:C	1:D:111:ASN:H	2.27	0.42
1:E:66:MET:CE	1:E:122:ALA:HB2	2.49	0.42
1:C:12:LEU:HD23	1:C:176:ASP:HB2	2.01	0.42
1:E:44:VAL:CG1	1:E:145:LEU:HD21	2.49	0.42
1:B:125:GLY:HA2	3:B:270:HOH:O	2.19	0.42
1:E:98:SER:HA	1:E:200:VAL:HG11	2.02	0.42
1:F:242:TYR:HA	1:F:243:PRO:HD3	1.71	0.42
1:A:24:ASN:HB2	1:A:25:PRO:HD3	2.02	0.42
1:A:91:ILE:HG12	1:A:127:ARG:HD3	2.01	0.42
3:A:453:HOH:O	1:B:220:LEU:C	2.63	0.42
1:B:153:ASP:HB2	3:B:424:HOH:O	2.20	0.42
1:D:97:ARG:HH21	1:D:201:GLU:CD	2.28	0.42
1:A:190:ASN:HD22	1:A:203:GLN:NE2	2.18	0.41
1:C:161:ILE:CD1	1:C:200:VAL:HG21	2.49	0.41
1:C:207:GLU:OE1	1:D:100:ARG:HD2	2.20	0.41
1:E:144:TYR:CE1	1:E:247:PRO:HG3	2.55	0.41
1:A:169:VAL:HG22	1:A:185:ALA:HB2	2.01	0.41
1:C:194:THR:HG21	1:D:210:THR:HG21	2.02	0.41
3:A:453:HOH:O	1:B:224:LEU:HD12	2.20	0.41
1:A:97:ARG:HH11	1:A:201:GLU:CD	2.28	0.41
1:B:23:GLU:HB2	1:F:121:GLN:HE22	1.85	0.41
1:C:77:ARG:HA	3:C:433:HOH:O	2.20	0.41
1:D:44:VAL:HG11	1:D:145:LEU:HD21	2.03	0.41
1:B:48:VAL:HG12	1:B:49:PRO:CD	2.49	0.41
1:F:107:ALA:HB1	1:F:153:ASP:CB	2.41	0.41
1:A:103:ILE:CD1	1:A:156:PRO:HB2	2.50	0.41
1:B:147:ALA:HB3	1:B:247:PRO:HD2	2.02	0.41
1:D:48:VAL:HG11	1:D:58:GLY:HA2	2.02	0.41
1:B:67:LEU:HD23	3:B:380:HOH:O	2.21	0.41
1:E:103:ILE:HD11	1:E:138:LEU:CD2	2.51	0.41
1:E:231:PHE:O	1:E:235:ARG:HG3	2.21	0.41
1:F:173:ILE:HD12	1:F:218:LYS:HB3	2.03	0.41
1:A:24:ASN:HB3	3:C:424:HOH:O	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:153:ASP:OD1	1:E:154:PRO:HD2	2.21	0.41
1:A:91:ILE:O	1:A:95:ILE:HG13	2.21	0.40
1:A:203:GLN:HE21	1:A:203:GLN:HB3	1.68	0.40
1:D:242:TYR:HA	1:D:243:PRO:HD3	1.83	0.40
1:D:245:VAL:HG12	1:D:246:LEU:N	2.35	0.40
1:F:44:VAL:CG1	1:F:145:LEU:HD21	2.50	0.40
1:F:125:GLY:HA2	3:F:266:HOH:O	2.20	0.40
1:F:153:ASP:CG	1:F:154:PRO:HD2	2.46	0.40
1:B:246:LEU:HA	1:B:247:PRO:HD3	1.92	0.40
1:B:24:ASN:HB2	1:B:25:PRO:HD3	2.03	0.40
1:A:153:ASP:HB3	3:A:459:HOH:O	2.21	0.40
1:C:32:GLU:HA	1:C:36:THR:O	2.22	0.40
1:C:188:ASP:O	1:C:205:THR:HA	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	239/262 (91%)	233 (98%)	6 (2%)	0	100	100
1	B	235/262 (90%)	233 (99%)	2 (1%)	0	100	100
1	C	237/262 (90%)	230 (97%)	6 (2%)	1 (0%)	30	28
1	D	235/262 (90%)	225 (96%)	8 (3%)	2 (1%)	14	10
1	E	236/262 (90%)	225 (95%)	8 (3%)	3 (1%)	9	6
1	F	236/262 (90%)	231 (98%)	5 (2%)	0	100	100
All	All	1418/1572 (90%)	1377 (97%)	35 (2%)	6 (0%)	30	28

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	245	VAL
1	D	8	LEU
1	E	46	GLU
1	C	49	PRO
1	E	109	GLY
1	E	245	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	188/203 (93%)	188 (100%)	0	100	100
1	B	186/203 (92%)	186 (100%)	0	100	100
1	C	188/203 (93%)	188 (100%)	0	100	100
1	D	186/203 (92%)	185 (100%)	1 (0%)	81	88
1	E	187/203 (92%)	187 (100%)	0	100	100
1	F	187/203 (92%)	186 (100%)	1 (0%)	81	88
All	All	1122/1218 (92%)	1120 (100%)	2 (0%)	87	93

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	127	ARG
1	F	177	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	121	GLN
1	A	190	ASN
1	A	203	GLN
1	B	72	HIS
1	B	111	ASN
1	B	190	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	35	HIS
1	C	111	ASN
1	C	121	GLN
1	C	203	GLN
1	D	190	ASN
1	D	203	GLN
1	E	121	GLN
1	E	190	ASN
1	F	190	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

10 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	259	-	4,4,4	0.96	0	6,6,6	0.46	0
2	PO4	D	260	-	4,4,4	0.97	0	6,6,6	0.46	0
2	PO4	F	260	-	4,4,4	0.96	0	6,6,6	0.44	0
2	PO4	C	260	-	4,4,4	1.01	0	6,6,6	0.57	0
2	PO4	A	259	-	4,4,4	0.94	0	6,6,6	0.47	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	PO4	D	259	-	4,4,4	0.95	0	6,6,6	0.47	0
2	PO4	C	259	-	4,4,4	0.95	0	6,6,6	0.45	0
2	PO4	E	259	-	4,4,4	0.96	0	6,6,6	0.47	0
2	PO4	F	259	-	4,4,4	0.94	0	6,6,6	0.46	0
2	PO4	A	260	-	4,4,4	0.95	0	6,6,6	0.51	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.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	260	PO4	1	0

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	243/262 (92%)	0.21	19 (7%) 19 20	17, 30, 64, 84	0
1	B	239/262 (91%)	0.31	22 (9%) 14 15	18, 31, 68, 86	0
1	C	241/262 (91%)	0.40	17 (7%) 22 23	20, 33, 66, 82	0
1	D	239/262 (91%)	0.65	26 (10%) 10 11	23, 38, 79, 95	0
1	E	240/262 (91%)	0.51	30 (12%) 8 8	23, 36, 72, 96	0
1	F	240/262 (91%)	0.50	20 (8%) 17 18	22, 35, 75, 90	0
All	All	1442/1572 (91%)	0.43	134 (9%) 14 15	17, 34, 72, 96	0

All (134) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	46	GLU	9.1
1	C	51	TRP	7.4
1	C	50	ARG	6.6
1	D	47	GLY	5.5
1	A	246	LEU	5.3
1	B	49	PRO	5.3
1	A	244	GLY	5.3
1	D	45	THR	5.2
1	E	57	LEU	4.9
1	D	245	VAL	4.9
1	A	49	PRO	4.8
1	F	49	PRO	4.8
1	D	57	LEU	4.7
1	C	49	PRO	4.6
1	A	245	VAL	4.5
1	D	49	PRO	4.4
1	A	54	ALA	4.3
1	D	48	VAL	4.3
1	D	247	PRO	4.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	49	PRO	4.2
1	C	5	ASP	4.1
1	F	57	LEU	4.1
1	B	48	VAL	4.1
1	A	57	LEU	4.0
1	B	107	ALA	4.0
1	E	48	VAL	4.0
1	B	4	GLU	3.9
1	B	57	LEU	3.8
1	F	188	ASP	3.8
1	F	48	VAL	3.8
1	F	108	LEU	3.7
1	B	209	ALA	3.7
1	E	111	ASN	3.7
1	A	48	VAL	3.7
1	B	206	GLY	3.6
1	A	106	ALA	3.6
1	D	246	LEU	3.5
1	C	206	GLY	3.5
1	E	206	GLY	3.5
1	E	245	VAL	3.5
1	B	246	LEU	3.4
1	F	245	VAL	3.4
1	D	44	VAL	3.4
1	B	208	GLY	3.3
1	F	206	GLY	3.3
1	C	245	VAL	3.3
1	F	106	ALA	3.3
1	D	154	PRO	3.2
1	B	245	VAL	3.2
1	C	148	ALA	3.2
1	D	108	LEU	3.1
1	D	152	SER	3.1
1	E	205	THR	3.1
1	D	151	LEU	3.1
1	E	246	LEU	3.1
1	C	57	LEU	3.0
1	D	149	GLY	3.0
1	F	148	ALA	3.0
1	D	107	ALA	2.9
1	F	107	ALA	2.9
1	E	58	GLY	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	45	THR	2.9
1	A	47	GLY	2.9
1	C	47	GLY	2.9
1	B	204	GLY	2.8
1	A	46	GLU	2.8
1	D	111	ASN	2.8
1	C	204	GLY	2.8
1	F	246	LEU	2.8
1	D	153	ASP	2.7
1	E	197	GLY	2.7
1	F	109	GLY	2.7
1	F	45	THR	2.7
1	A	56	GLY	2.7
1	C	208	GLY	2.7
1	E	46	GLU	2.6
1	A	112	THR	2.6
1	D	109	GLY	2.6
1	E	110	GLU	2.6
1	E	247	PRO	2.6
1	B	247	PRO	2.6
1	F	103	ILE	2.6
1	E	244	GLY	2.6
1	B	81	ARG	2.5
1	B	154	PRO	2.5
1	B	147	ALA	2.5
1	B	108	LEU	2.5
1	E	151	LEU	2.5
1	A	81	ARG	2.5
1	E	47	GLY	2.5
1	E	105	LEU	2.4
1	B	5	ASP	2.4
1	A	55	THR	2.4
1	A	108	LEU	2.4
1	B	106	ALA	2.4
1	F	47	GLY	2.4
1	D	112	THR	2.3
1	F	110	GLU	2.3
1	C	6	GLY	2.3
1	A	45	THR	2.3
1	A	83	ARG	2.3
1	E	106	ALA	2.3
1	B	109	GLY	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	208	GLY	2.3
1	E	108	LEU	2.3
1	E	103	ILE	2.2
1	D	244	GLY	2.2
1	E	208	GLY	2.2
1	F	244	GLY	2.2
1	E	147	ALA	2.2
1	D	145	LEU	2.2
1	C	72	HIS	2.2
1	E	196	THR	2.2
1	E	44	VAL	2.2
1	A	149	GLY	2.2
1	E	207	GLU	2.2
1	D	106	ALA	2.2
1	E	155	ARG	2.2
1	F	111	ASN	2.2
1	D	6	GLY	2.1
1	E	153	ASP	2.1
1	C	205	THR	2.1
1	B	244	GLY	2.1
1	B	105	LEU	2.1
1	C	108	LEU	2.1
1	E	240	LEU	2.1
1	D	144	TYR	2.1
1	D	242	TYR	2.1
1	F	83	ARG	2.1
1	E	243	PRO	2.1
1	E	109	GLY	2.1
1	B	45	THR	2.0
1	A	107	ALA	2.0
1	C	246	LEU	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(Å ²)	Q<0.9
2	PO4	A	259	5/5	0.76	0.11	52,61,69,76	0
2	PO4	F	260	5/5	0.79	0.11	52,59,66,72	0
2	PO4	C	259	5/5	0.86	0.10	51,61,62,67	0
2	PO4	D	259	5/5	0.88	0.08	49,57,61,68	0
2	PO4	D	260	5/5	0.94	0.10	28,34,41,45	0
2	PO4	E	259	5/5	0.96	0.07	30,31,36,36	0
2	PO4	A	260	5/5	0.96	0.08	26,31,36,44	0
2	PO4	F	259	5/5	0.97	0.07	26,28,37,38	0
2	PO4	C	260	5/5	0.99	0.04	26,26,31,33	0
2	PO4	B	259	5/5	0.99	0.04	24,24,25,26	0

6.5 Other polymers [i](#)

There are no such residues in this entry.