Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:53 PM GMT

PDB ID	:	4U7D
Title	:	Structure of human RECQ-like helicase in complex with an oligonucleotide
Authors	:	Pike, A.C.W.; Zhang, Y.; Schnecke, C.; Cooper, C.D.O.; Von Delft, F.; Arrowsmith, C.H.; Edwards, A.; Bountra, C.; Gileadi, O.; Structural Genomics Consortium (SGC)
Deposited on	:	2014-07-30
Resolution	:	3.40 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see references ①) were used in the production of this report:

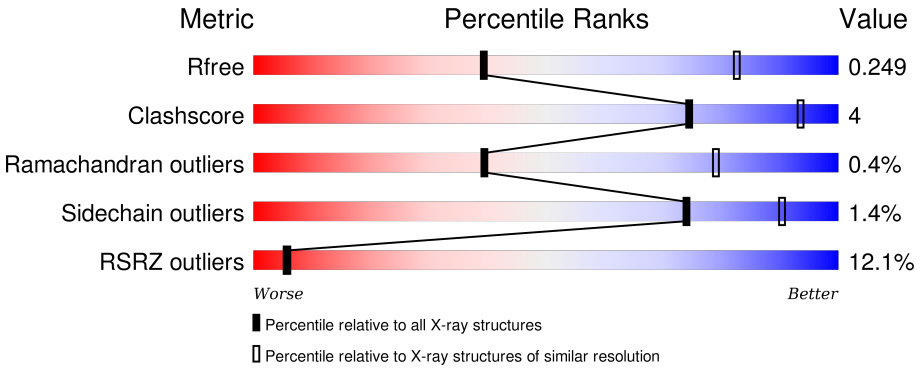
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 3.40 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.



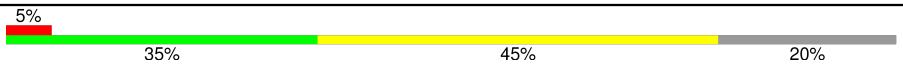
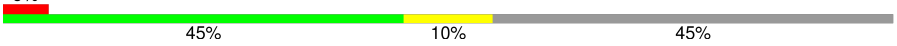
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1476 (3.50-3.30)
Clashscore	102246	1611 (3.50-3.30)
Ramachandran outliers	100387	1571 (3.50-3.30)
Sidechain outliers	100360	1571 (3.50-3.30)
RSRZ outliers	91569	1485 (3.50-3.30)

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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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	591	8% 80% 9% 11%
1	B	591	6% 79% 10% 11%
1	C	591	9% 81% 9% 10%
1	D	591	21% 81% 8% 10%
2	P	20	5% 30% 55% 15%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	Q	20	
2	R	20	
2	S	20	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 17224 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 ATP-dependent DNA helicase Q1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	527	Total	C	N	O	S	0	0	0
			4056	2594	678	751	33			
1	B	527	Total	C	N	O	S	0	0	0
			4052	2594	675	749	34			
1	C	530	Total	C	N	O	S	0	0	0
			4062	2601	677	751	33			
1	D	530	Total	C	N	O	S	0	0	0
			4070	2604	678	755	33			

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	48	MET	-	initiating methionine	UNP P46063
A	611	SER	GLY	conflict	UNP P46063
A	617	ALA	-	expression tag	UNP P46063
A	618	GLU	-	expression tag	UNP P46063
A	619	ASN	-	expression tag	UNP P46063
A	620	LEU	-	expression tag	UNP P46063
A	621	TYR	-	expression tag	UNP P46063
A	622	PHE	-	expression tag	UNP P46063
A	623	GLN	-	expression tag	UNP P46063
A	624	SER	-	expression tag	UNP P46063
A	625	HIS	-	expression tag	UNP P46063
A	626	HIS	-	expression tag	UNP P46063
A	627	HIS	-	expression tag	UNP P46063
A	628	HIS	-	expression tag	UNP P46063
A	629	HIS	-	expression tag	UNP P46063
A	630	HIS	-	expression tag	UNP P46063
A	631	ASP	-	expression tag	UNP P46063
A	632	TYR	-	expression tag	UNP P46063
A	633	LYS	-	expression tag	UNP P46063
A	634	ASP	-	expression tag	UNP P46063
A	635	ASP	-	expression tag	UNP P46063

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	636	ASP	-	expression tag	UNP P46063
A	637	ASP	-	expression tag	UNP P46063
A	638	LYS	-	expression tag	UNP P46063
B	48	MET	-	initiating methionine	UNP P46063
B	611	SER	GLY	conflict	UNP P46063
B	617	ALA	-	expression tag	UNP P46063
B	618	GLU	-	expression tag	UNP P46063
B	619	ASN	-	expression tag	UNP P46063
B	620	LEU	-	expression tag	UNP P46063
B	621	TYR	-	expression tag	UNP P46063
B	622	PHE	-	expression tag	UNP P46063
B	623	GLN	-	expression tag	UNP P46063
B	624	SER	-	expression tag	UNP P46063
B	625	HIS	-	expression tag	UNP P46063
B	626	HIS	-	expression tag	UNP P46063
B	627	HIS	-	expression tag	UNP P46063
B	628	HIS	-	expression tag	UNP P46063
B	629	HIS	-	expression tag	UNP P46063
B	630	HIS	-	expression tag	UNP P46063
B	631	ASP	-	expression tag	UNP P46063
B	632	TYR	-	expression tag	UNP P46063
B	633	LYS	-	expression tag	UNP P46063
B	634	ASP	-	expression tag	UNP P46063
B	635	ASP	-	expression tag	UNP P46063
B	636	ASP	-	expression tag	UNP P46063
B	637	ASP	-	expression tag	UNP P46063
B	638	LYS	-	expression tag	UNP P46063
C	48	MET	-	initiating methionine	UNP P46063
C	611	SER	GLY	conflict	UNP P46063
C	617	ALA	-	expression tag	UNP P46063
C	618	GLU	-	expression tag	UNP P46063
C	619	ASN	-	expression tag	UNP P46063
C	620	LEU	-	expression tag	UNP P46063
C	621	TYR	-	expression tag	UNP P46063
C	622	PHE	-	expression tag	UNP P46063
C	623	GLN	-	expression tag	UNP P46063
C	624	SER	-	expression tag	UNP P46063
C	625	HIS	-	expression tag	UNP P46063
C	626	HIS	-	expression tag	UNP P46063
C	627	HIS	-	expression tag	UNP P46063
C	628	HIS	-	expression tag	UNP P46063
C	629	HIS	-	expression tag	UNP P46063

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	630	HIS	-	expression tag	UNP P46063
C	631	ASP	-	expression tag	UNP P46063
C	632	TYR	-	expression tag	UNP P46063
C	633	LYS	-	expression tag	UNP P46063
C	634	ASP	-	expression tag	UNP P46063
C	635	ASP	-	expression tag	UNP P46063
C	636	ASP	-	expression tag	UNP P46063
C	637	ASP	-	expression tag	UNP P46063
C	638	LYS	-	expression tag	UNP P46063
D	48	MET	-	initiating methionine	UNP P46063
D	611	SER	GLY	conflict	UNP P46063
D	617	ALA	-	expression tag	UNP P46063
D	618	GLU	-	expression tag	UNP P46063
D	619	ASN	-	expression tag	UNP P46063
D	620	LEU	-	expression tag	UNP P46063
D	621	TYR	-	expression tag	UNP P46063
D	622	PHE	-	expression tag	UNP P46063
D	623	GLN	-	expression tag	UNP P46063
D	624	SER	-	expression tag	UNP P46063
D	625	HIS	-	expression tag	UNP P46063
D	626	HIS	-	expression tag	UNP P46063
D	627	HIS	-	expression tag	UNP P46063
D	628	HIS	-	expression tag	UNP P46063
D	629	HIS	-	expression tag	UNP P46063
D	630	HIS	-	expression tag	UNP P46063
D	631	ASP	-	expression tag	UNP P46063
D	632	TYR	-	expression tag	UNP P46063
D	633	LYS	-	expression tag	UNP P46063
D	634	ASP	-	expression tag	UNP P46063
D	635	ASP	-	expression tag	UNP P46063
D	636	ASP	-	expression tag	UNP P46063
D	637	ASP	-	expression tag	UNP P46063
D	638	LYS	-	expression tag	UNP P46063

- Molecule 2 is a DNA chain called DNA oligonucleotide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	P	17	Total	C	N	O	P	0	0	0
			323	154	54	99	16			
2	Q	16	Total	C	N	O	P	0	0	0
			311	149	54	93	15			
2	R	9	Total	C	N	O	P	0	0	0
			156	74	24	50	8			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	S	11	Total	C	N	O	P	0	0	0
			190	89	27	63	11			

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

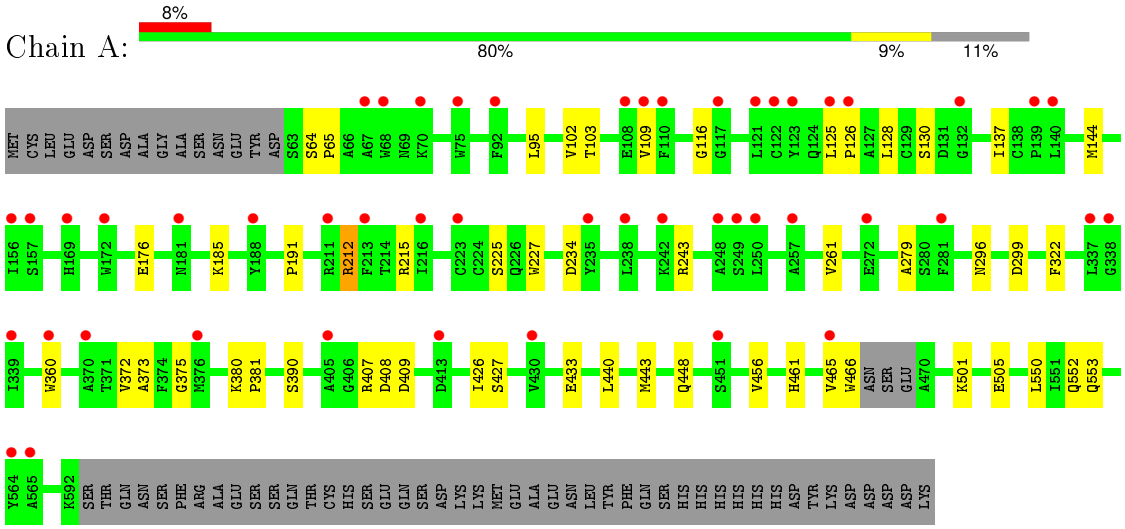
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Zn	0	0
			1	1		
3	A	1	Total	Zn	0	0
			1	1		
3	D	1	Total	Zn	0	0
			1	1		
3	C	1	Total	Zn	0	0
			1	1		

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 errors 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.

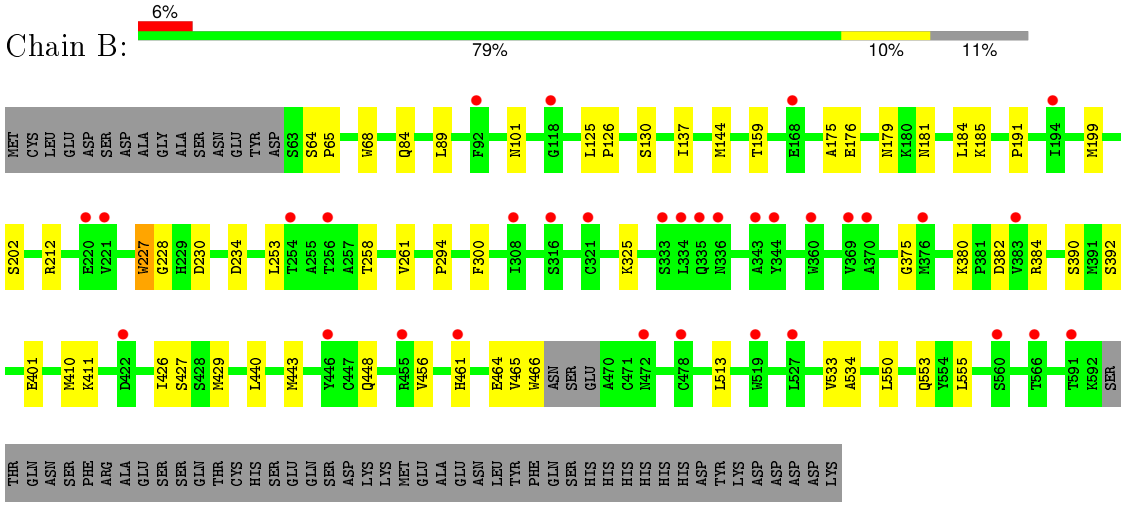
- Molecule 1: ATP-dependent DNA helicase Q1

Chain A:



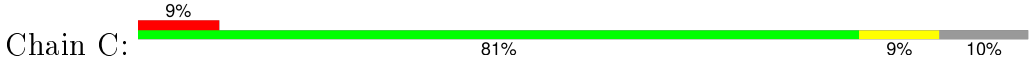
- Molecule 1: ATP-dependent DNA helicase Q1

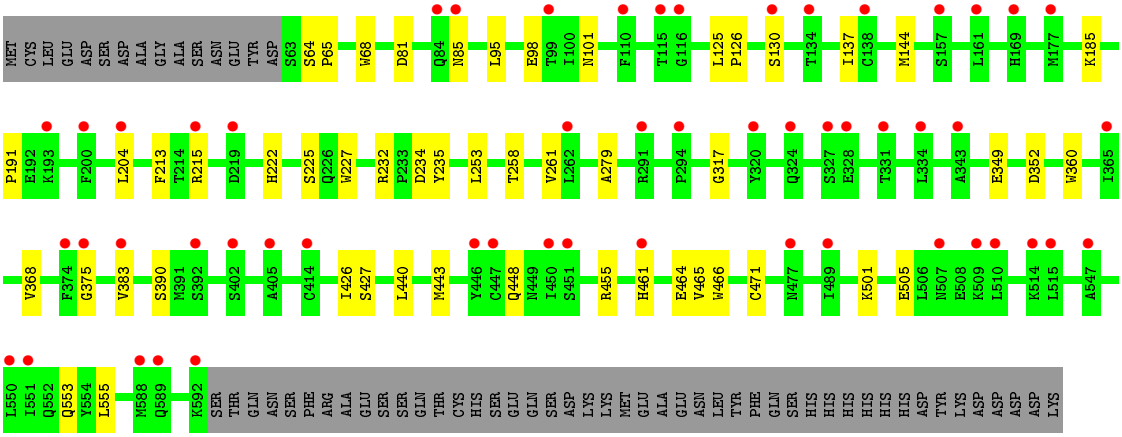
Chain B:



- Molecule 1: ATP-dependent DNA helicase Q1

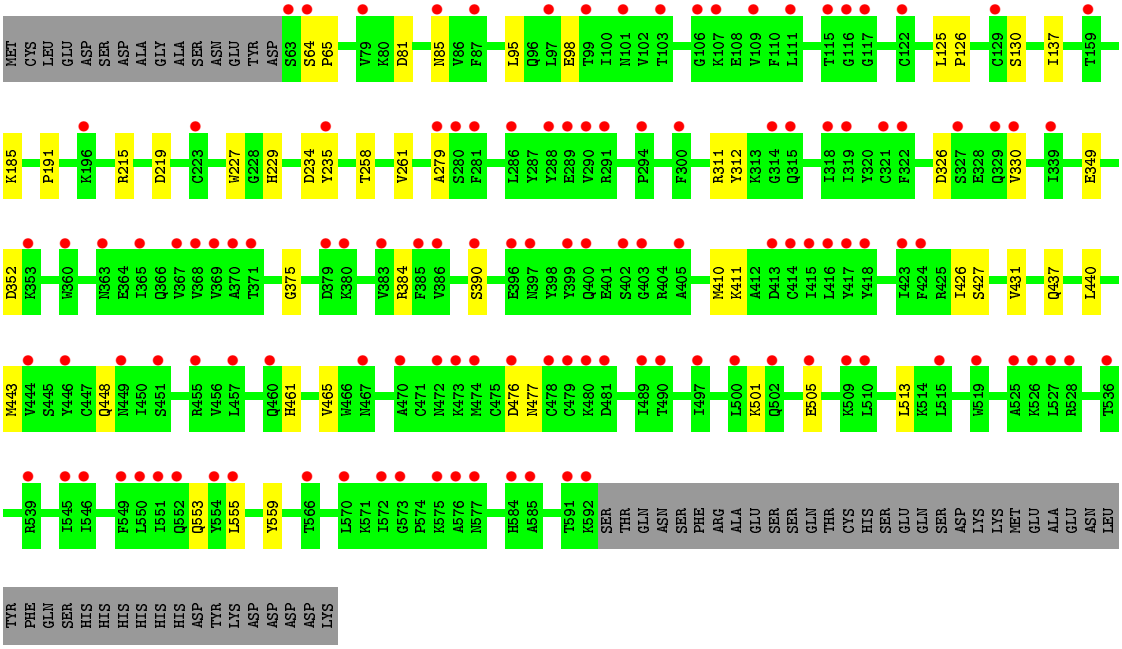
Chain C:





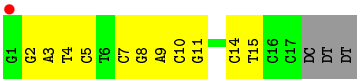
• Molecule 1: ATP-dependent DNA helicase Q1

Chain D:



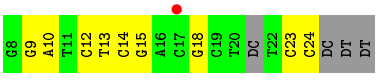
• Molecule 2: DNA oligonucleotide

Chain P:



• Molecule 2: DNA oligonucleotide

Chain Q:

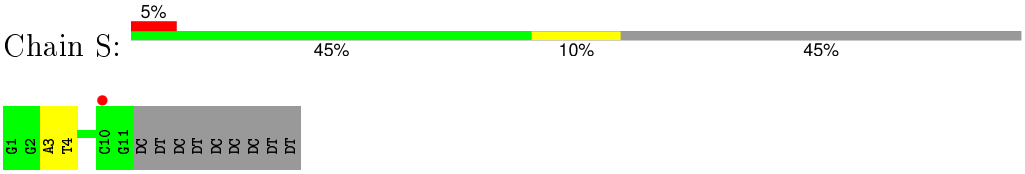


- Molecule 2: DNA oligonucleotide

Chain R:

- Molecule 2: DNA oligonucleotide

Chain S:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	55.38Å 138.22Å 207.58Å 90.00° 90.02° 90.00°	Depositor
Resolution (Å)	39.90 – 3.40 83.00 – 3.40	Depositor EDS
% Data completeness (in resolution range)	94.9 (39.90-3.40) 94.9 (83.00-3.40)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.93 (at 3.41Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1682)	Depositor
R, R_{free}	0.205 , 0.249 0.209 , 0.249	Depositor DCC
R_{free} test set	1888 reflections (4.84%)	DCC
Wilson B-factor (Å^2)	78.3	Xtriage
Anisotropy	0.315	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 48.7	EDS
Estimated twinning fraction	0.337 for h,-k,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.39$, $< L^2 > = 0.22$	Xtriage
Outliers	1 of 40943 reflections (0.002%)	Xtriage
F_o,F_c correlation	0.77	EDS
Total number of atoms	17224	wwPDB-VP
Average B, all atoms (Å^2)	94.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.67% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0.40	0/4137	0.58	0/5606
1	B	0.39	0/4133	0.61	0/5601
1	C	0.37	0/4144	0.57	0/5619
1	D	0.35	0/4152	0.56	0/5629
2	P	0.86	0/360	0.95	0/552
2	Q	0.85	0/346	0.91	0/529
2	R	0.71	0/172	0.96	0/262
2	S	0.62	0/211	0.91	0/322
All	All	0.42	0/17655	0.61	0/24120

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4056	0	3918	31	0
1	B	4052	0	3919	31	0
1	C	4062	0	3917	27	0
1	D	4070	0	3928	25	0
2	P	323	0	182	12	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	Q	311	0	174	9	0
2	R	156	0	88	4	0
2	S	190	0	104	2	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
All	All	17224	0	16230	130	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 4.

All (130) 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:130:SER:O	1:B:185:LYS:NZ	2.15	0.78
1:D:130:SER:O	1:D:185:LYS:NZ	2.22	0.72
1:A:130:SER:O	1:A:185:LYS:NZ	2.23	0.70
2:P:4:DT:O2	2:Q:18:DG:N2	2.30	0.64
1:A:243:ARG:NH2	1:D:431:VAL:O	2.26	0.64
1:C:130:SER:O	1:C:185:LYS:NZ	2.31	0.63
1:A:227:TRP:HB2	1:A:261:VAL:HG22	1.84	0.60
2:P:2:DG:C6	2:P:3:DA:C6	2.92	0.58
1:B:456:VAL:HG22	1:B:466:TRP:CD1	2.38	0.58
1:B:392:SER:OG	1:B:401:GLU:OE1	2.22	0.57
1:A:433:GLU:OE2	2:Q:23:DC:N4	2.38	0.57
1:A:373:ALA:HA	2:Q:24:DC:H4'	1.86	0.57
1:C:258:THR:HB	1:C:261:VAL:HG23	1.88	0.56
2:P:9:DA:C2	2:P:10:DC:N3	2.75	0.55
2:R:1:DG:N2	2:R:2:DG:N3	2.54	0.55
1:D:125:LEU:HB3	1:D:126:PRO:HD3	1.89	0.54
2:Q:14:DC:H2'	2:Q:15:DG:C8	2.44	0.53
1:B:325:LYS:HZ1	2:P:14:DC:P	2.31	0.53
1:A:130:SER:HB2	1:A:215:ARG:HH21	1.74	0.52
1:B:125:LEU:HB3	1:B:126:PRO:HD3	1.92	0.52
1:C:464:GLU:O	1:C:466:TRP:N	2.42	0.52
2:P:4:DT:H2"	2:P:5:DC:H5'	1.91	0.52
1:C:125:LEU:HB3	1:C:126:PRO:HD3	1.91	0.52
1:D:95:LEU:HD12	1:D:279:ALA:HA	1.90	0.52
1:B:513:LEU:HD13	2:Q:10:DA:H5'	1.91	0.52
2:Q:13:DT:H1'	2:Q:14:DC:H5'	1.93	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:426:ILE:HG21	1:D:440:LEU:HD13	1.91	0.51
1:A:381:PRO:HA	1:A:407:ARG:HB2	1.91	0.51
1:C:426:ILE:HG21	1:C:440:LEU:HD13	1.92	0.51
1:A:95:LEU:HD12	1:A:279:ALA:HA	1.93	0.50
1:A:176:GLU:O	1:A:212:ARG:NH2	2.43	0.50
2:P:9:DA:C2	2:Q:12:DC:N3	2.80	0.50
1:D:191:PRO:HB2	1:D:234:ASP:HB3	1.94	0.50
1:A:125:LEU:HB3	1:A:126:PRO:HD3	1.94	0.49
1:B:137:ILE:N	1:B:137:ILE:HD12	2.27	0.49
1:C:137:ILE:HD12	1:C:137:ILE:N	2.27	0.49
1:A:95:LEU:HD12	1:A:279:ALA:CA	2.42	0.49
1:C:95:LEU:HA	1:C:98:GLU:OE1	2.12	0.49
1:D:513:LEU:HD13	2:R:3:DA:H5'	1.95	0.48
1:D:81:ASP:OD1	1:D:85:ASN:ND2	2.47	0.48
1:C:553:GLN:HA	1:C:555:LEU:O	2.14	0.48
1:D:258:THR:HB	1:D:261:VAL:HG23	1.96	0.48
1:B:191:PRO:HB2	1:B:234:ASP:HB3	1.95	0.48
1:B:325:LYS:NZ	2:P:14:DC:OP1	2.39	0.47
1:B:426:ILE:HG21	1:B:440:LEU:HD13	1.96	0.47
2:P:10:DC:H2"	2:P:11:DG:H5'	1.96	0.47
1:A:137:ILE:N	1:A:137:ILE:HD12	2.30	0.47
1:D:227:TRP:CD1	1:D:227:TRP:N	2.82	0.47
1:B:84:GLN:HA	1:B:89:LEU:O	2.14	0.47
1:B:227:TRP:N	1:B:227:TRP:CD1	2.83	0.47
1:D:137:ILE:HD12	1:D:137:ILE:N	2.30	0.47
1:C:349:GLU:O	1:C:352:ASP:N	2.47	0.47
1:A:103:THR:O	1:A:215:ARG:NH1	2.47	0.47
1:D:384:ARG:NH1	1:D:410:MET:O	2.48	0.47
1:A:372:VAL:HG23	2:Q:24:DC:C5'	2.45	0.46
1:C:95:LEU:HD12	1:C:279:ALA:HA	1.98	0.46
1:C:68:TRP:O	1:C:101:ASN:ND2	2.44	0.46
1:B:294:PRO:HG2	1:B:300:PHE:HA	1.98	0.46
1:B:550:LEU:O	1:B:553:GLN:N	2.44	0.46
1:B:380:LYS:NZ	1:B:382:ASP:OD1	2.41	0.46
1:B:68:TRP:O	1:B:101:ASN:ND2	2.48	0.46
1:C:227:TRP:N	1:C:227:TRP:CD1	2.84	0.46
1:C:191:PRO:HB2	1:C:234:ASP:HB3	1.98	0.46
2:Q:9:DG:C6	2:Q:10:DA:N6	2.83	0.45
1:A:322:PHE:CE1	1:A:426:ILE:HG12	2.52	0.45
1:C:227:TRP:HB2	1:C:261:VAL:HG22	1.98	0.45
1:A:116:GLY:HA3	1:A:407:ARG:NH1	2.31	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:501:LYS:O	1:A:505:GLU:HG3	2.16	0.45
1:C:204:LEU:HD22	1:C:213:PHE:CE2	2.52	0.45
1:C:225:SER:HB3	1:C:261:VAL:HG13	1.98	0.45
1:C:95:LEU:HD12	1:C:279:ALA:CA	2.47	0.45
1:D:384:ARG:NE	1:D:411:LYS:O	2.44	0.45
1:C:455:ARG:HD2	1:C:471:CYS:SG	2.58	0.44
1:A:191:PRO:HB2	1:A:234:ASP:HB3	1.99	0.44
1:C:501:LYS:O	1:C:505:GLU:HG3	2.16	0.44
1:B:464:GLU:O	1:B:466:TRP:N	2.50	0.44
1:A:426:ILE:HG21	1:A:440:LEU:HD13	2.00	0.44
1:A:102:VAL:HG11	1:A:109:VAL:HB	1.98	0.44
1:C:81:ASP:OD1	1:C:85:ASN:ND2	2.51	0.43
1:D:476:ASP:OD2	1:D:477:ASN:N	2.52	0.43
1:D:95:LEU:HD12	1:D:279:ALA:CA	2.49	0.43
1:B:64:SER:HB2	1:B:65:PRO:HD2	1.99	0.43
1:A:64:SER:HB2	1:A:65:PRO:HD2	2.00	0.43
1:B:175:ALA:O	1:B:179:ASN:HB2	2.17	0.43
1:D:95:LEU:HA	1:D:98:GLU:OE1	2.19	0.43
1:C:317:GLY:HA2	1:C:383:VAL:HG13	2.00	0.43
1:C:360:TRP:CG	1:C:368:VAL:CG2	3.01	0.43
1:A:550:LEU:O	1:A:553:GLN:N	2.49	0.43
1:D:326:ASP:O	1:D:330:VAL:HG23	2.18	0.43
2:S:3:DA:H2"	2:S:4:DT:H5'	2.00	0.43
1:D:553:GLN:HA	1:D:555:LEU:O	2.19	0.43
1:D:130:SER:HB2	1:D:215:ARG:HH21	1.82	0.43
1:B:179:ASN:OD1	1:B:181:ASN:N	2.51	0.42
1:A:227:TRP:N	1:A:227:TRP:CD1	2.87	0.42
2:P:7:DC:H2'	2:P:8:DG:C8	2.54	0.42
1:B:258:THR:HB	1:B:261:VAL:HG23	2.01	0.42
1:A:225:SER:HB3	1:A:261:VAL:HG13	2.01	0.42
1:C:144:MET:HB2	1:C:144:MET:HE3	1.89	0.42
1:D:437:GLN:NE2	1:D:559:TYR:OH	2.49	0.42
1:B:384:ARG:NH1	1:B:410:MET:O	2.52	0.42
1:B:429:MET:CE	2:P:15:DT:H2"	2.49	0.42
1:B:199:MET:O	1:B:202:SER:OG	2.34	0.42
1:D:219:ASP:O	1:D:235:TYR:OH	2.29	0.42
1:D:501:LYS:O	1:D:505:GLU:HG3	2.19	0.42
1:A:408:ASP:O	1:A:409:ASP:HB2	2.20	0.42
2:P:4:DT:H2"	2:P:5:DC:C5'	2.50	0.41
1:C:232:ARG:O	1:C:235:TYR:HB2	2.19	0.41
2:P:11:DG:H2'	2:P:11:DG:N3	2.34	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:64:SER:HB2	1:C:65:PRO:HD2	2.02	0.41
1:D:64:SER:HB2	1:D:65:PRO:HD2	2.02	0.41
1:A:296:ASN:HB3	1:A:299:ASP:HB2	2.03	0.41
1:D:349:GLU:O	1:D:352:ASP:N	2.48	0.41
2:S:3:DA:H1'	2:S:4:DT:C5'	2.51	0.41
1:B:159:THR:CG2	1:B:184:LEU:HD21	2.50	0.41
1:A:128:LEU:HA	1:A:185:LYS:HD2	2.03	0.41
2:R:1:DG:C2	2:R:2:DG:C4	3.08	0.41
1:B:553:GLN:HA	1:B:555:LEU:O	2.21	0.41
1:B:384:ARG:NE	1:B:411:LYS:O	2.43	0.41
1:B:228:GLY:O	1:B:230:ASP:N	2.53	0.41
1:A:456:VAL:HG22	1:A:466:TRP:CD1	2.56	0.41
1:C:222:HIS:HB2	1:C:261:VAL:HG11	2.03	0.41
1:B:144:MET:HB2	1:B:144:MET:HE2	1.94	0.41
1:A:552:GLN:O	1:A:553:GLN:HB2	2.21	0.40
1:A:360:TRP:CH2	1:A:380:LYS:HD3	2.56	0.40
1:A:144:MET:HE3	1:A:144:MET:HB2	1.90	0.40
1:D:311:ARG:HD2	1:D:312:TYR:CZ	2.56	0.40
1:B:176:GLU:O	1:B:212:ARG:NH2	2.54	0.40
1:C:130:SER:HB2	1:C:215:ARG:HH21	1.86	0.40
2:R:12:DC:H2'	2:R:13:DT:H71	2.03	0.40
1:B:533:VAL:HG12	1:B:534:ALA:O	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	523/591 (88%)	499 (95%)	22 (4%)	2 (0%)	39	79
1	B	523/591 (88%)	500 (96%)	21 (4%)	2 (0%)	39	79
1	C	528/591 (89%)	504 (96%)	22 (4%)	2 (0%)	39	79

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	D	528/591 (89%)	503 (95%)	22 (4%)	3 (1%)	30 72
All	All	2102/2364 (89%)	2006 (95%)	87 (4%)	9 (0%)	39 79

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	465	VAL
1	A	375	GLY
1	A	465	VAL
1	B	375	GLY
1	B	465	VAL
1	C	375	GLY
1	D	229	HIS
1	D	375	GLY
1	D	465	VAL

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	416/521 (80%)	410 (99%)	6 (1%)	74 90
1	B	416/521 (80%)	409 (98%)	7 (2%)	68 88
1	C	414/521 (80%)	408 (99%)	6 (1%)	74 90
1	D	417/521 (80%)	412 (99%)	5 (1%)	78 91
All	All	1663/2084 (80%)	1639 (99%)	24 (1%)	74 90

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	212	ARG
1	A	390	SER
1	A	427	SER
1	A	443	MET
1	A	448	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	461	HIS
1	B	227	TRP
1	B	253	LEU
1	B	390	SER
1	B	427	SER
1	B	443	MET
1	B	448	GLN
1	B	461	HIS
1	C	253	LEU
1	C	390	SER
1	C	427	SER
1	C	443	MET
1	C	448	GLN
1	C	461	HIS
1	D	390	SER
1	D	427	SER
1	D	443	MET
1	D	448	GLN
1	D	461	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	357	HIS
1	A	389	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 carbohydrates in this entry.

5.6 Ligand geometry

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

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

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, 95^{th} 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	527/591 (89%)	0.74	49 (9%) 11 11	42, 82, 133, 160	0
1	B	527/591 (89%)	0.67	33 (6%) 23 22	52, 78, 110, 131	0
1	C	530/591 (89%)	0.79	54 (10%) 9 9	66, 96, 134, 158	0
1	D	530/591 (89%)	1.26	124 (23%) 1 1	60, 116, 153, 168	0
2	P	17/20 (85%)	0.84	1 (5%) 26 23	78, 99, 108, 111	0
2	Q	16/20 (80%)	0.72	1 (6%) 23 22	71, 92, 107, 108	0
2	R	9/20 (45%)	0.00	0 100 100	127, 134, 136, 139	0
2	S	11/20 (55%)	0.70	1 (9%) 11 11	109, 131, 137, 140	0
All	All	2167/2444 (88%)	0.86	263 (12%) 6 6	42, 89, 140, 168	0

All (263) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	416	LEU	8.8
1	D	480	LYS	8.2
1	D	510	LEU	6.7
1	D	370	ALA	6.6
1	D	417	TYR	6.4
1	D	288	TYR	6.4
1	D	365	ILE	6.0
1	D	451	SER	6.0
1	C	343	ALA	5.9
1	D	591	THR	5.4
1	D	300	PHE	5.4
1	D	554	TYR	5.3
1	B	254	THR	5.1
1	D	570	LEU	5.1
1	A	70	LYS	4.9
1	D	106	GLY	4.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	344	TYR	4.7
1	C	510	LEU	4.6
1	C	392	SER	4.6
1	D	592	LYS	4.6
1	C	138	CYS	4.6
1	D	415	ILE	4.6
1	D	424	PHE	4.5
1	B	168	GLU	4.5
1	D	371	THR	4.4
1	D	403	GLY	4.4
1	D	481	ASP	4.4
1	D	460	GLN	4.3
1	D	400	GLN	4.2
1	C	116	GLY	4.2
1	D	575	LYS	4.1
1	A	564	TYR	4.1
1	D	546	ILE	4.1
1	D	472	ASN	4.1
1	C	402	SER	4.1
1	D	402	SER	4.0
1	D	502	GLN	4.0
1	D	576	ALA	4.0
1	C	451	SER	4.0
1	D	314	GLY	4.0
1	A	108	GLU	4.0
1	B	360	TRP	4.0
1	A	216	ILE	3.9
1	D	291	ARG	3.8
1	D	235	TYR	3.8
1	D	363	ASN	3.8
1	D	396	GLU	3.8
1	B	376	MET	3.8
1	D	327	SER	3.7
1	A	122	CYS	3.7
1	D	85	ASN	3.7
1	A	75	TRP	3.6
1	A	67	ALA	3.6
1	A	451	SER	3.6
1	D	368	VAL	3.6
1	B	455	ARG	3.6
1	B	335	GLN	3.5
1	D	527	LEU	3.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	211	ARG	3.5
1	C	130	SER	3.5
1	C	447	CYS	3.5
1	D	103	THR	3.5
1	D	490	THR	3.5
1	B	343	ALA	3.5
1	D	519	TRP	3.4
1	D	111	LEU	3.4
1	D	115	THR	3.4
1	D	584	HIS	3.4
1	A	250	LEU	3.4
1	B	336	ASN	3.4
1	B	383	VAL	3.4
1	D	509	LYS	3.3
1	C	215	ARG	3.3
1	D	281	PHE	3.3
1	D	423	ILE	3.3
1	C	200	PHE	3.2
1	A	249	SER	3.2
1	D	525	ALA	3.2
1	D	555	LEU	3.2
1	C	589	GLN	3.2
1	C	405	ALA	3.2
1	C	85	ASN	3.2
1	B	334	LEU	3.2
1	D	457	LEU	3.2
1	C	592	LYS	3.2
1	D	322	PHE	3.2
1	A	465	VAL	3.2
1	D	585	ALA	3.2
1	C	115	THR	3.1
1	D	116	GLY	3.1
1	D	223	CYS	3.1
1	D	505	GLU	3.1
1	D	315	GLN	3.1
1	C	477	ASN	3.1
1	D	467	ASN	3.1
1	D	101	ASN	3.1
1	C	99	THR	3.0
1	A	370	ALA	3.0
1	A	238	LEU	3.0
1	D	449	ASN	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	290	VAL	3.0
1	A	188	TYR	3.0
1	A	338	GLY	3.0
1	D	87	PHE	3.0
1	D	545	ILE	3.0
1	D	413	ASP	2.9
1	A	126	PRO	2.9
1	A	281	PHE	2.9
1	D	479	CYS	2.9
1	C	446	TYR	2.9
1	D	446	TYR	2.9
1	D	369	VAL	2.9
1	D	286	LEU	2.9
1	A	157	SER	2.9
1	B	221	VAL	2.9
1	B	321	CYS	2.9
1	C	193	LYS	2.9
1	D	399	TYR	2.9
1	A	109	VAL	2.8
1	B	333	SER	2.8
1	A	68	TRP	2.8
1	A	257	ALA	2.8
1	A	125	LEU	2.8
2	S	10	DC	2.8
1	D	497	ILE	2.8
1	D	379	ASP	2.7
1	D	380	LYS	2.7
1	B	308	ILE	2.7
1	D	572	ILE	2.7
1	C	331	THR	2.7
1	C	547	ALA	2.7
1	A	156	ILE	2.7
1	B	220	GLU	2.7
1	A	235	TYR	2.7
1	A	376	MET	2.7
1	A	172	TRP	2.7
1	D	418	TYR	2.7
1	C	550	LEU	2.7
1	D	279	ALA	2.7
1	D	64	SER	2.6
1	C	588	MET	2.6
1	A	213	PHE	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	370	ALA	2.6
1	D	551	ILE	2.6
1	A	132	GLY	2.6
1	B	256	THR	2.6
1	D	339	ILE	2.6
1	D	470	ALA	2.6
1	D	549	PHE	2.6
1	D	383	VAL	2.6
1	D	474	MET	2.6
1	C	169	HIS	2.6
1	A	248	ALA	2.5
1	D	566	THR	2.5
1	B	527	LEU	2.5
1	B	194	ILE	2.5
1	C	515	LEU	2.5
1	D	515	LEU	2.5
1	C	177	MET	2.5
1	A	181	ASN	2.5
1	D	405	ALA	2.5
1	C	334	LEU	2.5
1	C	375	GLY	2.5
2	P	1	DG	2.5
1	A	169	HIS	2.5
1	C	204	LEU	2.5
1	B	472	ASN	2.5
1	D	79	VAL	2.5
1	D	385	PHE	2.5
1	C	324	GLN	2.5
1	D	489	ILE	2.5
1	B	591	THR	2.4
1	C	450	ILE	2.4
1	A	565	ALA	2.4
1	B	446	TYR	2.4
1	C	157	SER	2.4
1	C	514	LYS	2.4
1	D	294	PRO	2.4
1	D	97	LEU	2.4
1	D	552	GLN	2.4
1	D	577	ASN	2.4
1	D	478	CYS	2.4
1	A	92	PHE	2.4
1	C	291	ARG	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	455	ARG	2.4
1	D	289	GLU	2.4
1	A	242	LYS	2.4
1	A	123	TYR	2.4
1	D	386	VAL	2.4
1	D	159	THR	2.3
1	B	461	HIS	2.3
1	A	337	LEU	2.3
1	D	414	CYS	2.3
1	A	121	LEU	2.3
1	A	430	VAL	2.3
1	C	551	ILE	2.3
1	C	320	TYR	2.3
1	D	129	CYS	2.3
1	D	353	LYS	2.3
1	C	262	LEU	2.3
1	A	110	PHE	2.3
1	B	92	PHE	2.3
1	D	318	ILE	2.3
1	C	327	SER	2.3
1	B	316	SER	2.3
1	C	414	CYS	2.3
1	D	63	SER	2.3
1	D	539	ARG	2.2
1	D	526	LYS	2.2
1	D	280	SER	2.2
1	C	328	GLU	2.2
1	D	397	ASN	2.2
1	C	383	VAL	2.2
1	D	330	VAL	2.2
1	C	507	ASN	2.2
1	D	196	LYS	2.2
1	D	473	LYS	2.2
1	B	422	ASP	2.2
1	A	223	CYS	2.2
1	D	321	CYS	2.2
1	D	476	ASP	2.2
1	C	374	PHE	2.2
1	C	509	LYS	2.2
1	A	272	GLU	2.2
1	C	134	THR	2.2
1	A	139	PRO	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	99	THR	2.2
1	D	528	ARG	2.2
1	A	405	ALA	2.2
1	A	140	LEU	2.2
1	C	161	LEU	2.2
1	D	500	LEU	2.2
1	A	360	TRP	2.2
1	D	390	SER	2.2
1	B	118	GLY	2.2
1	C	294	PRO	2.2
1	B	369	VAL	2.2
1	D	367	VAL	2.2
1	B	519	TRP	2.1
1	D	109	VAL	2.1
1	D	360	TRP	2.1
1	C	365	ILE	2.1
1	D	107	LYS	2.1
1	D	319	ILE	2.1
1	A	117	GLY	2.1
1	C	219	ASP	2.1
1	C	110	PHE	2.1
1	C	461	HIS	2.1
1	C	84	GLN	2.1
1	D	536	THR	2.1
1	B	560	SER	2.1
1	A	413	ASP	2.1
1	C	489	ILE	2.1
1	D	329	GLN	2.1
1	D	550	LEU	2.1
1	D	444	VAL	2.1
1	A	339	ILE	2.0
2	Q	17	DC	2.0
1	B	566	THR	2.0
1	D	573	GLY	2.0
1	B	478	CYS	2.0
1	D	122	CYS	2.0
1	D	117	GLY	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 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} 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	LLDF	B-factors(Å^2)	Q<0.9
3	ZN	A	701	1/1	0.97	0.14	-1.01	75,75,75,75	0
3	ZN	C	701	1/1	0.97	0.14	-1.12	94,94,94,94	0
3	ZN	D	701	1/1	0.96	0.08	-2.01	131,131,131,131	0
3	ZN	B	701	1/1	0.94	0.12	-2.22	91,91,91,91	0

6.5 Other polymers (i)

There are no such residues in this entry.