



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:12 AM GMT

PDB ID : 2G1T
Title : A Src-like Inactive Conformation in the Abl Tyrosine Kinase Domain
Authors : Levinson, N.M.; Kuchment, O.
Deposited on : 2006-02-14
Resolution : 1.80 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 ⓘ](#)) 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

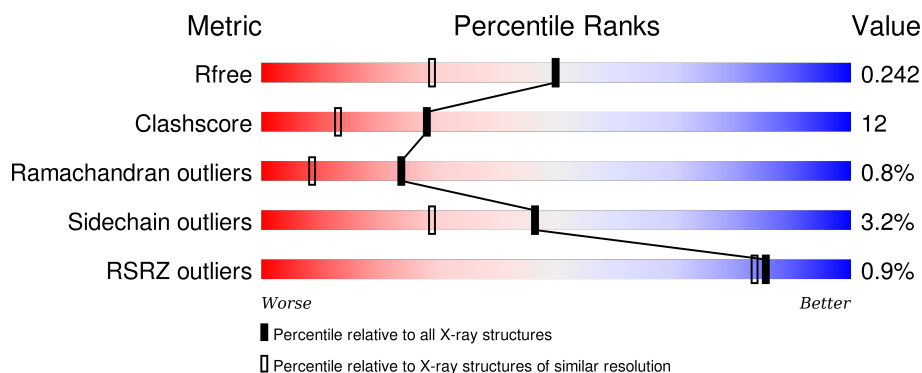
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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.




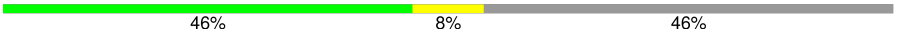

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	4533 (1.80-1.80)
Clashscore	102246	5383 (1.80-1.80)
Ramachandran outliers	100387	5320 (1.80-1.80)
Sidechain outliers	100360	5319 (1.80-1.80)
RSRZ outliers	91569	4547 (1.80-1.80)

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 $\leq 5\%$. 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	287	<div> <div>2%</div> <div>78% 15% • 6%</div> </div>
1	B	287	<div> <div>71% 22% • 5%</div> </div>
1	C	287	<div> <div>71% 24% • •</div> </div>
1	D	287	<div> <div>2%</div> <div>79% 15% • •</div> </div>
2	E	13	<div> <div>62% 38%</div> </div>

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Mol	Chain	Length	Quality of chain
2	F	13	 62% 8% 8% 23%
2	G	13	 46% 8% 46%
2	H	13	 54% 8% 38%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 10249 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 Proto-oncogene tyrosine-protein kinase ABL1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	271	Total	C	N	O	S	0	0	0
			2210	1424	359	410	17			
1	B	273	Total	C	N	O	S	0	0	0
			2225	1433	362	413	17			
1	C	276	Total	C	N	O	S	0	0	0
			2249	1446	364	422	17			
1	D	277	Total	C	N	O	S	0	0	0
			2253	1449	368	418	18			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	226	GLY	-	CLONING ARTIFACT	UNP P00519
A	227	HIS	-	CLONING ARTIFACT	UNP P00519
A	228	MET	-	CLONING ARTIFACT	UNP P00519
B	226	GLY	-	CLONING ARTIFACT	UNP P00519
B	227	HIS	-	CLONING ARTIFACT	UNP P00519
B	228	MET	-	CLONING ARTIFACT	UNP P00519
C	226	GLY	-	CLONING ARTIFACT	UNP P00519
C	227	HIS	-	CLONING ARTIFACT	UNP P00519
C	228	MET	-	CLONING ARTIFACT	UNP P00519
D	226	GLY	-	CLONING ARTIFACT	UNP P00519
D	227	HIS	-	CLONING ARTIFACT	UNP P00519
D	228	MET	-	CLONING ARTIFACT	UNP P00519

- Molecule 2 is a protein called ATP-Peptide Conjugate.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	8	Total	C	N	O	0	0	0
			66	44	8	14			
2	F	10	Total	C	N	O	0	0	0
			76	50	10	16			

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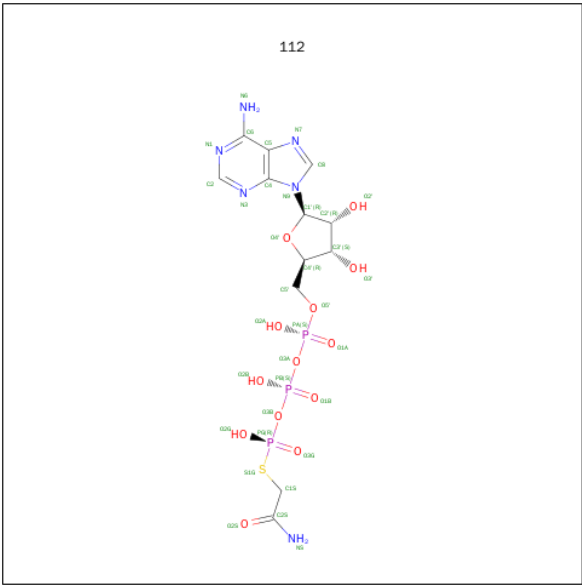
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	G	7	Total	C	N	O	0	0	0
			57	39	7	11			
2	H	8	Total	C	N	O	0	0	0
			70	46	8	16			

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 4 is THIOPHOSPHORIC ACID O-((ADENOSYL-PHOSPHO)PHOSPHO)-S-AC ETAMIDYL-DIESTER (three-letter code: 112) (formula: C₁₂H₁₉N₆O₁₃P₃S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	E	1	Total	C	N	O	P	S	0	0
			35	12	6	13	3	1		
4	F	1	Total	C	N	O	P	S	0	0
			35	12	6	13	3	1		
4	G	1	Total	C	N	O	P	S	0	0
			35	12	6	13	3	1		

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	H	1	Total	C	N	O	P	S	0	0
			35	12	6	13	3	1		

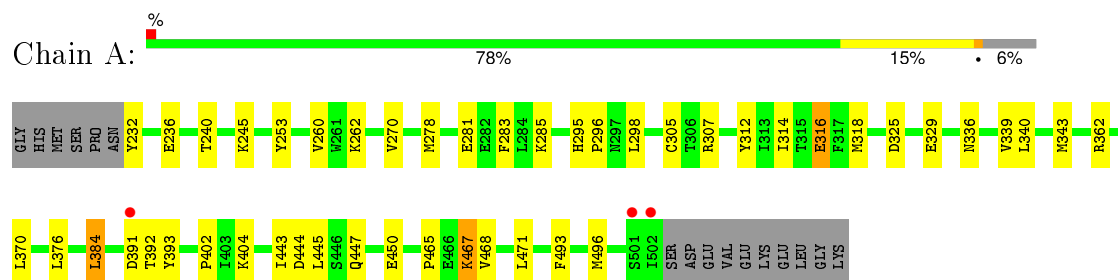
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	244	Total	O	0	0
			244	244		
5	B	197	Total	O	0	0
			197	197		
5	C	172	Total	O	0	0
			172	172		
5	D	209	Total	O	0	0
			209	209		
5	E	19	Total	O	0	0
			19	19		
5	F	29	Total	O	0	0
			29	29		
5	G	15	Total	O	0	0
			15	15		
5	H	14	Total	O	0	0
			14	14		

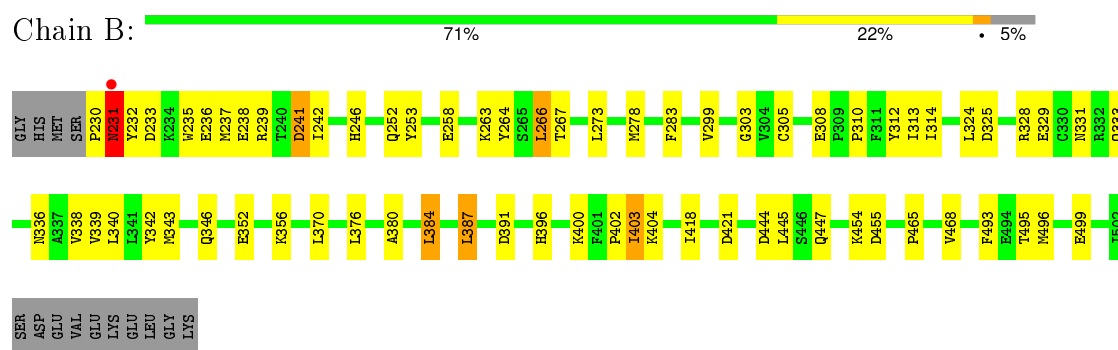
3 Residue-property plots [i](#)

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.

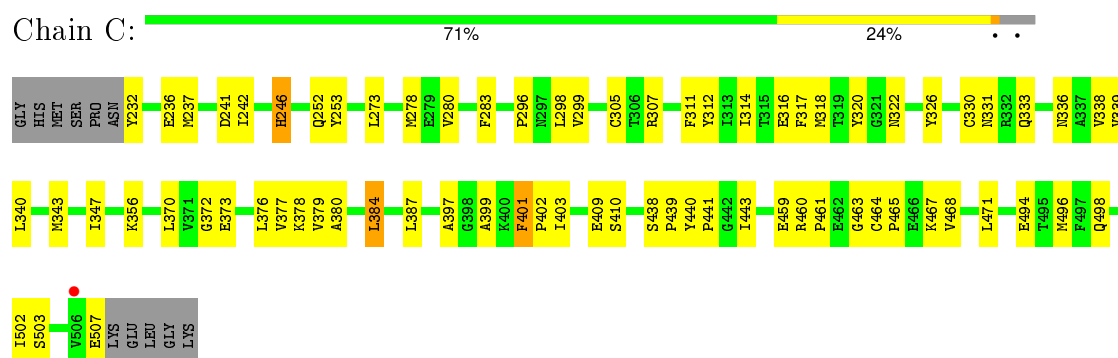
- Molecule 1: Proto-oncogene tyrosine-protein kinase ABL1



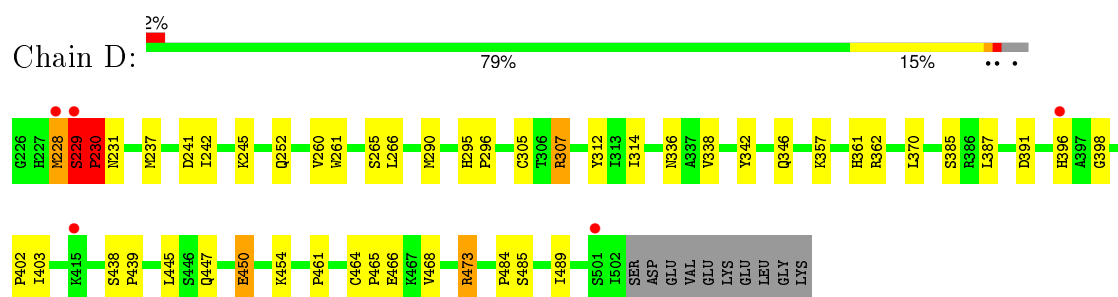
- Molecule 1: Proto-oncogene tyrosine-protein kinase ABL1



- Molecule 1: Proto-oncogene tyrosine-protein kinase ABL1



- Molecule 1: Proto-oncogene tyrosine-protein kinase ABL1



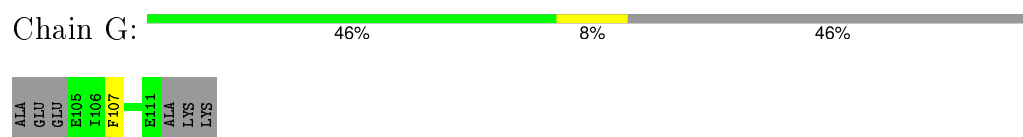
- Molecule 2: ATP-Peptide Conjugate



- Molecule 2: ATP-Peptide Conjugate



- Molecule 2: ATP-Peptide Conjugate



- Molecule 2: ATP-Peptide Conjugate



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	62.59Å 78.44Å 141.61Å 90.00° 90.11° 90.00°	Depositor
Resolution (Å)	50.00 – 1.80 48.92 – 1.83	Depositor EDS
% Data completeness (in resolution range)	92.6 (50.00-1.80) 96.9 (48.92-1.83)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.90 (at 1.83Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.219 , 0.244 0.214 , 0.242	Depositor DCC
R_{free} test set	11279 reflections (9.59%)	DCC
Wilson B-factor (Å ²)	21.8	Xtriage
Anisotropy	0.824	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 30.3	EDS
Estimated twinning fraction	0.084 for h,-k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Outliers	0 of 117589 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	10249	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.08% 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, 0.375 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: MG, 112

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	0.33	0/2267	0.62	1/3068 (0.0%)
1	B	0.32	0/2283	0.60	1/3090 (0.0%)
1	C	0.31	0/2306	0.58	1/3121 (0.0%)
1	D	0.35	0/2312	0.61	2/3129 (0.1%)
2	E	0.50	0/67	0.55	0/88
2	F	0.48	0/77	0.57	0/102
2	G	0.49	0/58	0.65	0/76
2	H	0.48	0/71	0.50	0/93
All	All	0.33	0/9441	0.60	5/12767 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	402	PRO	N-CA-C	-6.78	94.47	112.10
1	B	402	PRO	N-CA-C	-6.65	94.81	112.10
1	D	402	PRO	N-CA-C	-5.67	97.36	112.10
1	C	402	PRO	N-CA-C	-5.32	98.28	112.10
1	D	229	SER	N-CA-C	5.31	125.33	111.00

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	2210	0	2163	34	0
1	B	2225	0	2177	61	0
1	C	2249	0	2193	71	0
1	D	2253	0	2200	50	0
2	E	66	0	54	0	0
2	F	76	0	58	3	0
2	G	57	0	45	1	0
2	H	70	0	55	1	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
4	E	35	0	14	0	0
4	F	35	0	14	0	0
4	G	35	0	14	0	0
4	H	35	0	15	1	0
5	A	244	0	0	4	0
5	B	197	0	0	1	0
5	C	172	0	0	1	0
5	D	209	0	0	3	0
5	E	19	0	0	0	0
5	F	29	0	0	0	0
5	G	15	0	0	0	0
5	H	14	0	0	1	0
All	All	10249	0	9002	215	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 12.

All (215) 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:D:307:ARG:HH11	1:D:307:ARG:HB2	1.08	1.15
1:D:473:ARG:HB3	1:D:473:ARG:HH11	1.33	0.94
1:C:278:MET:HE1	1:C:283:PHE:HD1	1.34	0.91
1:D:307:ARG:HH11	1:D:307:ARG:CB	1.87	0.86
1:D:484:PRO:HG2	1:D:489:ILE:HD11	1.58	0.86
1:D:307:ARG:HB2	1:D:307:ARG:NH1	1.93	0.84
1:B:237:MET:HE3	1:B:314:ILE:HD13	1.60	0.82
1:C:237:MET:HE1	1:C:314:ILE:HB	1.64	0.80
1:A:404:LYS:HE3	1:A:445:LEU:HD23	1.65	0.78
1:C:316:GLU:OE2	1:C:318:MET:HE1	1.87	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:278:MET:CE	1:B:283:PHE:HD1	1.99	0.74
1:C:278:MET:CE	1:C:283:PHE:HD1	2.03	0.72
1:C:237:MET:HE3	1:C:314:ILE:HD13	1.72	0.71
1:B:324:LEU:O	1:B:328:ARG:HG2	1.89	0.71
1:A:340:LEU:HA	1:A:343:MET:HE2	1.74	0.69
1:B:273:LEU:HD13	1:B:313:ILE:HD13	1.74	0.69
1:B:278:MET:HE2	1:B:387:LEU:O	1.93	0.68
1:D:336:ASN:OD1	1:D:338:VAL:HG12	1.93	0.68
1:D:484:PRO:CG	1:D:489:ILE:HD11	2.24	0.68
1:D:237:MET:HE2	1:D:242:ILE:HD11	1.77	0.67
1:A:447:GLN:HG2	1:C:459:GLU:OE2	1.95	0.67
1:A:443:ILE:HD13	1:C:441:PRO:O	1.95	0.67
1:C:336:ASN:OD1	1:C:339:VAL:HG23	1.96	0.66
1:B:493:PHE:HA	1:B:496:MET:HE3	1.76	0.66
1:D:229:SER:O	1:D:230:PRO:C	2.31	0.66
1:A:340:LEU:HD23	1:A:343:MET:HE1	1.78	0.65
1:D:445:LEU:HD12	1:D:445:LEU:H	1.60	0.65
1:D:485:SER:O	1:D:489:ILE:HD13	1.96	0.64
1:D:473:ARG:HB3	1:D:473:ARG:NH1	2.11	0.64
1:B:305:CYS:HB2	1:B:312:TYR:HB2	1.79	0.64
1:A:391:ASP:O	1:A:391:ASP:OD1	2.16	0.63
1:B:238:GLU:HB2	1:B:241:ASP:OD1	1.98	0.63
1:B:352:GLU:O	1:B:356:LYS:HG3	1.98	0.63
5:A:1691:HOH:O	1:D:228:MET:HG3	1.99	0.63
1:B:312:TYR:C	1:B:313:ILE:HD12	2.20	0.63
1:C:376:LEU:HD11	1:C:378:LYS:HG3	1.80	0.62
1:D:242:ILE:N	1:D:242:ILE:HD12	2.14	0.62
1:C:336:ASN:OD1	1:C:338:VAL:HG12	2.01	0.61
1:C:278:MET:HE1	1:C:283:PHE:CD1	2.25	0.61
1:D:461:PRO:HG2	1:D:464:CYS:HB2	1.83	0.61
1:D:245:LYS:HE3	1:D:260:VAL:CG2	2.31	0.61
1:C:252:GLN:HG3	2:G:107:PHE:CZ	2.36	0.60
1:B:242:ILE:N	1:B:242:ILE:HD12	2.15	0.59
1:A:316:GLU:HG3	1:A:318:MET:HE3	1.83	0.59
1:B:230:PRO:O	1:B:231:ASN:HB3	2.02	0.59
1:B:340:LEU:HA	1:B:343:MET:HE2	1.83	0.59
1:C:305:CYS:HB2	1:C:312:TYR:HB2	1.85	0.59
1:C:443:ILE:N	1:C:443:ILE:HD12	2.17	0.59
1:A:232:TYR:HB2	1:A:236:GLU:OE2	2.03	0.58
1:C:471:LEU:HD11	1:C:496:MET:HE1	1.84	0.58
1:D:237:MET:CE	1:D:242:ILE:HD11	2.33	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:305:CYS:HB2	1:A:312:TYR:HB2	1.86	0.58
1:D:245:LYS:HE3	1:D:260:VAL:HG23	1.85	0.57
1:B:495:THR:O	1:B:499:GLU:HG2	2.04	0.57
1:B:444:ASP:HB3	1:B:447:GLN:HE21	1.70	0.57
1:B:313:ILE:HD12	1:B:313:ILE:N	2.19	0.56
1:C:465:PRO:HG2	1:C:468:VAL:CG2	2.35	0.56
1:B:314:ILE:N	1:B:314:ILE:HD12	2.20	0.56
1:C:340:LEU:HD23	1:C:343:MET:HE1	1.86	0.56
1:C:347:ILE:HD11	1:C:377:VAL:CG1	2.36	0.56
1:D:362:ARG:HD3	1:D:385:SER:OG	2.06	0.56
1:B:339:VAL:O	1:B:343:MET:HG3	2.05	0.56
1:C:471:LEU:HD11	1:C:496:MET:CE	2.36	0.56
1:C:326:TYR:O	1:C:330:CYS:HB3	2.06	0.56
1:C:242:ILE:HD12	1:C:242:ILE:N	2.20	0.55
1:C:336:ASN:CG	1:C:338:VAL:HG12	2.25	0.55
1:B:237:MET:HE1	1:B:314:ILE:HB	1.88	0.55
1:D:314:ILE:N	1:D:314:ILE:HD12	2.20	0.55
1:C:299:VAL:HG21	1:C:380:ALA:HB2	1.88	0.55
1:D:229:SER:O	1:D:231:ASN:N	2.40	0.54
1:C:331:ASN:OD1	1:C:333:GLN:HB2	2.07	0.54
1:B:237:MET:HE3	1:B:314:ILE:CD1	2.36	0.54
1:C:307:ARG:HG3	1:C:307:ARG:HH11	1.72	0.54
1:B:325:ASP:HB3	1:B:329:GLU:OE2	2.07	0.54
1:B:263:LYS:HE3	1:B:264:TYR:CZ	2.43	0.54
1:A:325:ASP:O	1:A:329:GLU:HG3	2.07	0.53
1:C:347:ILE:HD11	1:C:377:VAL:HG11	1.91	0.53
1:C:322:ASN:HA	1:C:370:LEU:HD23	1.89	0.53
1:C:503:SER:O	1:C:507:GLU:HG3	2.08	0.53
1:C:314:ILE:HD12	1:C:314:ILE:N	2.24	0.53
1:B:273:LEU:CD1	1:B:313:ILE:HD13	2.39	0.53
1:C:343:MET:O	1:C:347:ILE:HG12	2.09	0.53
1:B:239:ARG:HH11	1:B:239:ARG:HG3	1.74	0.53
1:B:278:MET:CE	1:B:283:PHE:CD1	2.89	0.53
1:D:252:GLN:HG2	5:H:1413:HOH:O	2.09	0.52
1:B:396:HIS:NE2	2:F:109:GLU:HG3	2.24	0.52
1:C:340:LEU:HA	1:C:343:MET:HE2	1.91	0.52
1:B:278:MET:HE3	1:B:283:PHE:HB2	1.92	0.52
1:D:447:GLN:HA	1:D:447:GLN:NE2	2.25	0.51
1:C:278:MET:HE2	1:C:387:LEU:O	2.09	0.51
1:B:278:MET:HE1	1:B:283:PHE:HD1	1.72	0.51
1:B:336:ASN:OD1	1:B:338:VAL:HG12	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:278:MET:HE3	1:C:283:PHE:HB2	1.92	0.50
1:A:316:GLU:HG3	1:A:318:MET:CE	2.41	0.50
1:A:465:PRO:HG2	1:A:468:VAL:CG2	2.41	0.50
1:B:241:ASP:HB2	1:B:242:ILE:HD12	1.93	0.50
1:B:336:ASN:OD1	1:B:339:VAL:HG23	2.12	0.50
1:A:493:PHE:HA	1:A:496:MET:HE3	1.93	0.50
1:C:356:LYS:HE2	5:C:1763:HOH:O	2.11	0.50
1:C:376:LEU:C	1:C:376:LEU:HD13	2.32	0.50
1:B:253:TYR:CD2	1:B:384:LEU:HD13	2.47	0.50
1:C:316:GLU:HG3	1:C:318:MET:CE	2.42	0.49
1:C:336:ASN:ND2	1:C:338:VAL:HG12	2.27	0.49
1:D:357:LYS:HE3	5:D:1950:HOH:O	2.12	0.49
1:B:231:ASN:HD22	1:B:231:ASN:C	2.15	0.49
1:C:461:PRO:HG2	1:C:464:CYS:HB2	1.93	0.49
1:B:331:ASN:OD1	1:B:333:GLN:HB2	2.13	0.49
1:A:316:GLU:OE2	1:A:318:MET:HE1	2.13	0.49
1:D:473:ARG:CB	1:D:473:ARG:HH11	2.16	0.48
1:D:447:GLN:HA	1:D:447:GLN:HE21	1.78	0.48
1:B:266:LEU:HD22	1:B:267:THR:O	2.13	0.48
1:C:494:GLU:O	1:C:498:GLN:HG3	2.13	0.48
1:D:450:GLU:O	1:D:454:LYS:HG2	2.12	0.48
1:B:230:PRO:HB3	1:B:232:TYR:CE2	2.49	0.48
1:D:445:LEU:CD1	1:D:445:LEU:H	2.26	0.48
1:C:280:VAL:HG22	1:C:311:PHE:CZ	2.49	0.48
1:C:298:LEU:HD23	1:C:379:VAL:HB	1.95	0.47
1:A:340:LEU:CD2	1:A:343:MET:HE1	2.44	0.47
1:B:237:MET:CE	1:B:314:ILE:HD13	2.37	0.47
1:C:237:MET:CE	1:C:314:ILE:HD13	2.42	0.47
1:C:340:LEU:CD2	1:C:343:MET:HE1	2.45	0.47
1:D:237:MET:HE3	1:D:261:TRP:CE2	2.49	0.47
1:B:356:LYS:HE2	5:B:1797:HOH:O	2.14	0.47
1:D:241:ASP:HB2	1:D:242:ILE:HD12	1.96	0.46
1:D:307:ARG:HH11	1:D:307:ARG:CG	2.28	0.46
1:D:450:GLU:OE1	1:D:450:GLU:HA	2.15	0.46
1:B:299:VAL:HG21	1:B:380:ALA:HB2	1.97	0.46
1:C:441:PRO:O	1:C:443:ILE:HD12	2.15	0.46
1:B:352:GLU:HG2	1:B:356:LYS:HE3	1.97	0.46
1:D:362:ARG:NH1	5:D:1839:HOH:O	2.41	0.46
1:B:263:LYS:HE3	1:B:264:TYR:CE1	2.50	0.46
1:B:454:LYS:O	1:B:455:ASP:HB2	2.14	0.46
1:C:316:GLU:HG3	1:C:318:MET:HE3	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:316:GLU:CG	1:A:318:MET:HE3	2.46	0.45
1:A:467:LYS:HD2	1:A:467:LYS:N	2.31	0.45
1:C:299:VAL:HG13	1:C:316:GLU:HG2	1.98	0.45
1:C:399:ALA:HB3	1:C:401:PHE:CZ	2.51	0.45
1:A:392:THR:HG22	1:A:393:TYR:CE2	2.51	0.45
1:C:241:ASP:HB2	1:C:242:ILE:HD12	1.99	0.45
1:A:318:MET:HA	1:A:318:MET:HE2	1.98	0.45
1:C:336:ASN:OD1	1:C:338:VAL:CG1	2.64	0.45
1:A:281:GLU:O	1:A:285:LYS:HG3	2.17	0.45
1:B:465:PRO:HG2	1:B:468:VAL:CG2	2.46	0.45
1:A:339:VAL:O	1:A:343:MET:HG3	2.17	0.45
1:D:229:SER:HB2	1:D:230:PRO:HD3	1.98	0.45
1:D:228:MET:HB2	5:D:1987:HOH:O	2.15	0.45
1:C:278:MET:CE	1:C:283:PHE:CD1	2.92	0.44
1:C:278:MET:CE	1:C:387:LEU:O	2.65	0.44
1:A:336:ASN:OD1	1:A:339:VAL:HG23	2.17	0.44
1:B:252:GLN:HG3	2:F:107:PHE:CZ	2.52	0.44
1:C:409:GLU:HG2	1:C:410:SER:N	2.33	0.44
1:D:241:ASP:C	1:D:242:ILE:HD12	2.38	0.44
4:H:1401:112:H8	4:H:1401:112:H5'2	2.00	0.44
1:A:253:TYR:CD1	1:A:384:LEU:HD13	2.53	0.44
1:D:290:MET:SD	1:D:387:LEU:HD11	2.58	0.44
1:A:295:HIS:CG	1:A:296:PRO:HD2	2.53	0.44
1:C:317:PHE:O	1:C:318:MET:HE2	2.18	0.44
1:C:253:TYR:CD1	1:C:384:LEU:HD13	2.53	0.43
1:A:240:THR:HG23	5:A:1663:HOH:O	2.17	0.43
1:C:376:LEU:HD13	1:C:377:VAL:N	2.33	0.43
1:C:232:TYR:O	1:C:236:GLU:HG3	2.18	0.43
1:D:229:SER:O	1:D:231:ASN:ND2	2.51	0.43
1:C:376:LEU:CD1	1:C:378:LYS:HG3	2.47	0.43
1:D:447:GLN:CA	1:D:447:GLN:HE21	2.32	0.43
1:A:245:LYS:HE3	1:A:260:VAL:HG23	1.99	0.43
1:A:444:ASP:HB2	1:A:447:GLN:HG3	2.00	0.43
1:B:231:ASN:ND2	1:B:233:ASP:OD2	2.51	0.43
1:A:232:TYR:O	1:A:236:GLU:HG3	2.18	0.43
1:C:241:ASP:C	1:C:242:ILE:HD12	2.38	0.43
1:D:305:CYS:HB2	1:D:312:TYR:HB2	2.01	0.43
1:B:278:MET:HE3	1:B:283:PHE:HD1	1.80	0.43
1:B:246:HIS:HE1	1:B:258:GLU:OE2	2.01	0.43
1:C:467:LYS:HD3	1:C:496:MET:HG2	2.00	0.43
1:B:342:TYR:O	1:B:346:GLN:HG3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:245:LYS:HE3	1:D:260:VAL:HG21	2.00	0.43
1:A:262:LYS:NZ	5:A:1728:HOH:O	2.51	0.42
1:C:460:ARG:HD2	1:C:464:CYS:O	2.19	0.42
1:C:320:TYR:HD2	1:C:372:GLY:O	2.02	0.42
1:A:270:VAL:HG22	1:A:314:ILE:HD12	2.00	0.42
1:B:232:TYR:O	1:B:236:GLU:HG3	2.19	0.42
1:C:307:ARG:NH1	1:C:307:ARG:HG3	2.34	0.42
1:B:239:ARG:NH1	1:B:239:ARG:HG3	2.34	0.42
1:B:239:ARG:NH2	1:B:308:GLU:O	2.52	0.42
1:B:404:LYS:HE3	1:B:445:LEU:HD23	2.00	0.42
1:A:278:MET:HE1	1:A:283:PHE:HA	2.00	0.42
1:D:398:GLY:CA	2:H:111:GLU:HA	2.50	0.42
1:D:445:LEU:HD12	1:D:445:LEU:N	2.29	0.42
1:C:439:PRO:O	1:C:440:TYR:C	2.58	0.42
1:C:237:MET:HE3	1:C:314:ILE:CD1	2.43	0.42
1:D:342:TYR:O	1:D:346:GLN:HG3	2.20	0.42
1:B:273:LEU:HD22	1:B:313:ILE:HD11	2.02	0.42
1:B:403:ILE:HB	1:B:445:LEU:HD22	2.02	0.41
1:C:438:SER:HA	1:C:439:PRO:HD3	1.88	0.41
1:C:465:PRO:HG2	1:C:468:VAL:HG23	2.01	0.41
1:D:229:SER:HB2	1:D:230:PRO:CD	2.50	0.41
1:B:239:ARG:NH2	1:B:310:PRO:O	2.53	0.41
1:B:313:ILE:N	1:B:313:ILE:CD1	2.84	0.41
1:C:498:GLN:O	1:C:502:ILE:HG12	2.20	0.41
1:D:465:PRO:HG2	1:D:468:VAL:CG2	2.50	0.41
1:C:296:PRO:O	1:C:378:LYS:HE2	2.19	0.41
1:D:295:HIS:CG	1:D:296:PRO:HD2	2.55	0.41
1:B:235:TRP:HB2	1:B:303:GLY:HA2	2.03	0.41
1:A:307:ARG:HB2	1:A:307:ARG:HE	1.73	0.41
1:D:336:ASN:OD1	1:D:338:VAL:CG1	2.64	0.41
1:A:295:HIS:HB3	1:A:298:LEU:HD12	2.02	0.41
1:A:450:GLU:HG2	5:A:1715:HOH:O	2.21	0.41
1:D:438:SER:HA	1:D:439:PRO:HD3	1.94	0.41
1:B:232:TYR:HB3	1:B:235:TRP:CE2	2.56	0.41
1:D:361:HIS:O	1:D:362:ARG:CB	2.69	0.40
1:C:246:HIS:H	1:C:246:HIS:CD2	2.39	0.40
1:C:347:ILE:HD11	1:C:377:VAL:HG12	2.03	0.40
1:B:418:ILE:O	1:B:421:ASP:HB2	2.21	0.40
1:C:468:VAL:O	1:C:471:LEU:HB2	2.21	0.40
1:B:400:LYS:HA	2:F:109:GLU:HA	2.03	0.40
1:B:278:MET:HE3	1:B:283:PHE:CD1	2.56	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	269/287 (94%)	260 (97%)	9 (3%)	0	100	100
1	B	271/287 (94%)	261 (96%)	8 (3%)	2 (1%)	26	11
1	C	274/287 (96%)	265 (97%)	6 (2%)	3 (1%)	17	5
1	D	275/287 (96%)	262 (95%)	9 (3%)	4 (2%)	13	3
2	E	6/13 (46%)	6 (100%)	0	0	100	100
2	F	8/13 (62%)	8 (100%)	0	0	100	100
2	G	5/13 (38%)	5 (100%)	0	0	100	100
2	H	6/13 (46%)	6 (100%)	0	0	100	100
All	All	1114/1200 (93%)	1073 (96%)	32 (3%)	9 (1%)	24	8

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	397	ALA
1	D	229	SER
1	B	231	ASN
1	D	228	MET
1	D	230	PRO
1	C	403	ILE
1	B	403	ILE
1	D	403	ILE
1	C	463	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	237/251 (94%)	230 (97%)	7 (3%)	48	31
1	B	239/251 (95%)	231 (97%)	8 (3%)	45	27
1	C	242/251 (96%)	237 (98%)	5 (2%)	61	47
1	D	242/251 (96%)	232 (96%)	10 (4%)	37	19
2	E	6/10 (60%)	6 (100%)	0	100	100
2	F	6/10 (60%)	5 (83%)	1 (17%)	3	0
2	G	5/10 (50%)	5 (100%)	0	100	100
2	H	7/10 (70%)	7 (100%)	0	100	100
All	All	984/1044 (94%)	953 (97%)	31 (3%)	46	29

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	316	GLU
1	A	362	ARG
1	A	370	LEU
1	A	376	LEU
1	A	384	LEU
1	A	467	LYS
1	A	471	LEU
1	B	231	ASN
1	B	241	ASP
1	B	266	LEU
1	B	370	LEU
1	B	376	LEU
1	B	384	LEU
1	B	387	LEU
1	B	391	ASP
1	C	246	HIS
1	C	273	LEU
1	C	373	GLU
1	C	384	LEU
1	C	401	PHE
1	D	230	PRO
1	D	265	SER
1	D	266	LEU

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Mol	Chain	Res	Type
1	D	307	ARG
1	D	370	LEU
1	D	391	ASP
1	D	396	HIS
1	D	450	GLU
1	D	466	GLU
1	D	473	ARG
2	F	109	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	498	GLN
1	B	231	ASN
1	B	246	HIS
1	B	300	GLN
1	B	375	HIS
1	B	447	GLN
1	C	358	ASN
1	C	447	GLN
1	D	375	HIS
1	D	447	GLN
1	D	491	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 for Mogul analysis.

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
4	112	E	1101	3,2	25,37,37	2.05	7 (28%)	31,57,57	2.42	11 (35%)
4	112	F	1201	3,2	25,37,37	1.95	7 (28%)	31,57,57	2.35	10 (32%)
4	112	G	1301	3,2	25,37,37	2.06	7 (28%)	31,57,57	2.34	10 (32%)
4	112	H	1401	3,2	25,37,37	2.06	8 (32%)	31,57,57	2.48	9 (29%)

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
4	112	E	1101	3,2	-	0/18/44/44	0/3/3/3
4	112	F	1201	3,2	-	0/18/44/44	0/3/3/3
4	112	G	1301	3,2	-	0/18/44/44	0/3/3/3
4	112	H	1401	3,2	-	0/18/44/44	0/3/3/3

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	G	1301	112	PG-O2G	-4.10	1.45	1.56
4	E	1101	112	PG-O2G	-4.08	1.45	1.56
4	F	1201	112	PG-O2G	-3.98	1.46	1.56
4	H	1401	112	PG-O2G	-3.81	1.46	1.56
4	H	1401	112	O5'-C5'	-2.57	1.34	1.44
4	F	1201	112	O5'-C5'	-2.39	1.35	1.44
4	G	1301	112	O5'-C5'	-2.39	1.35	1.44
4	E	1101	112	O5'-C5'	-2.37	1.35	1.44
4	H	1401	112	C8-N7	-2.06	1.30	1.34
4	H	1401	112	C5-C4	2.26	1.45	1.40
4	F	1201	112	C5-C4	2.39	1.45	1.40
4	E	1101	112	C5-C4	2.41	1.45	1.40
4	G	1301	112	C5-C4	2.49	1.46	1.40
4	H	1401	112	C6-N6	2.71	1.43	1.34
4	E	1101	112	C6-N6	2.75	1.43	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	1201	112	C2-N1	2.85	1.39	1.33
4	F	1201	112	C6-N6	3.01	1.44	1.34
4	E	1101	112	C2-N3	3.10	1.37	1.32
4	G	1301	112	C6-N6	3.10	1.44	1.34
4	E	1101	112	C2-N1	3.11	1.39	1.33
4	G	1301	112	C2-N1	3.13	1.39	1.33
4	F	1201	112	C2-N3	3.19	1.37	1.32
4	H	1401	112	C2-N1	3.27	1.40	1.33
4	H	1401	112	C2-N3	3.34	1.38	1.32
4	G	1301	112	C2-N3	3.76	1.38	1.32
4	F	1201	112	C4-N3	4.67	1.42	1.35
4	G	1301	112	C4-N3	4.75	1.42	1.35
4	H	1401	112	C4-N3	5.13	1.43	1.35
4	E	1101	112	C4-N3	5.37	1.43	1.35

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	1101	112	O3A-PA-O5'	-5.51	88.31	102.94
4	H	1401	112	O3A-PA-O5'	-5.38	88.65	102.94
4	H	1401	112	N3-C2-N1	-5.17	124.94	128.89
4	E	1101	112	N3-C2-N1	-5.13	124.97	128.89
4	F	1201	112	O3A-PA-O5'	-5.12	89.35	102.94
4	G	1301	112	O3A-PA-O5'	-5.08	89.45	102.94
4	G	1301	112	N3-C2-N1	-5.06	125.02	128.89
4	F	1201	112	N3-C2-N1	-4.64	125.34	128.89
4	H	1401	112	O5'-PA-O1A	-2.68	99.20	109.62
4	E	1101	112	O5'-PA-O1A	-2.43	100.18	109.62
4	G	1301	112	O5'-PA-O1A	-2.40	100.29	109.62
4	H	1401	112	O2S-C2S-NS	-2.37	115.65	122.46
4	F	1201	112	O5'-PA-O1A	-2.25	100.87	109.62
4	F	1201	112	O2S-C2S-NS	-2.25	116.02	122.46
4	E	1101	112	O2S-C2S-NS	-2.23	116.06	122.46
4	G	1301	112	O2S-C2S-NS	-2.19	116.17	122.46
4	E	1101	112	C5'-C4'-C3'	-2.11	106.83	115.21
4	E	1101	112	O2A-PA-O1A	2.01	123.43	112.53
4	F	1201	112	O2A-PA-O1A	2.02	123.49	112.53
4	G	1301	112	O4'-C4'-C3'	2.09	109.36	105.15
4	F	1201	112	O4'-C4'-C3'	2.10	109.38	105.15
4	G	1301	112	O2A-PA-O1A	2.12	124.01	112.53
4	H	1401	112	O2A-PA-O1A	2.18	124.35	112.53
4	E	1101	112	O4'-C4'-C3'	2.20	109.57	105.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	1201	112	O2A-PA-O5'	2.33	120.20	108.46
4	G	1301	112	O2A-PA-O5'	2.52	121.15	108.46
4	E	1101	112	O2A-PA-O5'	2.60	121.57	108.46
4	H	1401	112	O2A-PA-O5'	2.62	121.69	108.46
4	G	1301	112	PA-O3A-PB	3.18	141.67	132.73
4	F	1201	112	PA-O3A-PB	3.34	142.12	132.73
4	F	1201	112	C4-C5-N7	3.76	112.94	109.48
4	E	1101	112	PA-O3A-PB	3.77	143.31	132.73
4	H	1401	112	PA-O3A-PB	3.82	143.47	132.73
4	E	1101	112	C4-C5-N7	4.00	113.16	109.48
4	G	1301	112	C4-C5-N7	4.03	113.19	109.48
4	H	1401	112	C4-C5-N7	4.25	113.39	109.48
4	G	1301	112	C1S-C2S-NS	7.04	123.24	115.48
4	E	1101	112	C1S-C2S-NS	7.39	123.63	115.48
4	F	1201	112	C1S-C2S-NS	7.78	124.06	115.48
4	H	1401	112	C1S-C2S-NS	7.82	124.09	115.48

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
4	H	1401	112	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	271/287 (94%)	-0.27	3 (1%) 82 80	13, 23, 43, 66	0
1	B	273/287 (95%)	-0.19	1 (0%) 93 91	13, 27, 45, 70	0
1	C	276/287 (96%)	-0.13	1 (0%) 93 91	18, 28, 49, 66	0
1	D	277/287 (96%)	-0.21	5 (1%) 71 67	15, 24, 45, 70	0
2	E	8/13 (61%)	0.18	0 100 100	22, 28, 37, 39	0
2	F	10/13 (76%)	-0.03	0 100 100	23, 33, 44, 44	0
2	G	7/13 (53%)	0.15	0 100 100	28, 30, 45, 45	0
2	H	8/13 (61%)	0.49	0 100 100	23, 44, 48, 51	0
All	All	1130/1200 (94%)	-0.19	10 (0%) 85 83	13, 26, 46, 70	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	501	SER	4.7
1	D	229	SER	4.4
1	B	231	ASN	3.5
1	C	506	VAL	3.5
1	A	391	ASP	3.2
1	D	501	SER	2.5
1	D	228	MET	2.3
1	D	415	LYS	2.3
1	A	502	ILE	2.1
1	D	396	HIS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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, 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	LLDF	B-factors(\AA^2)	Q<0.9
4	112	F	1201	35/35	0.97	0.10	1.03	20,24,27,30	0
4	112	H	1401	35/35	0.97	0.10	0.56	15,19,26,27	0
4	112	G	1301	35/35	0.97	0.10	0.55	18,24,28,29	0
4	112	E	1101	35/35	0.97	0.10	0.45	15,21,28,30	0
3	MG	C	1701	1/1	0.99	0.13	-	20,20,20,20	0
3	MG	D	1801	1/1	0.98	0.09	-	20,20,20,20	0
3	MG	B	1601	1/1	0.99	0.08	-	21,21,21,21	0
3	MG	A	1501	1/1	0.99	0.06	-	17,17,17,17	0

6.5 Other polymers [i](#)

There are no such residues in this entry.