Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 01:02 PM GMT

PDB ID	:	3SJA
Title	:	Crystal structure of S. cerevisiae Get3 in the open state in complex with Get1 cytosolic domain
Authors	:	Reitz, S.; Wild, K.; Sinning, I.
Deposited on	:	2011-06-21
Resolution	:	3.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

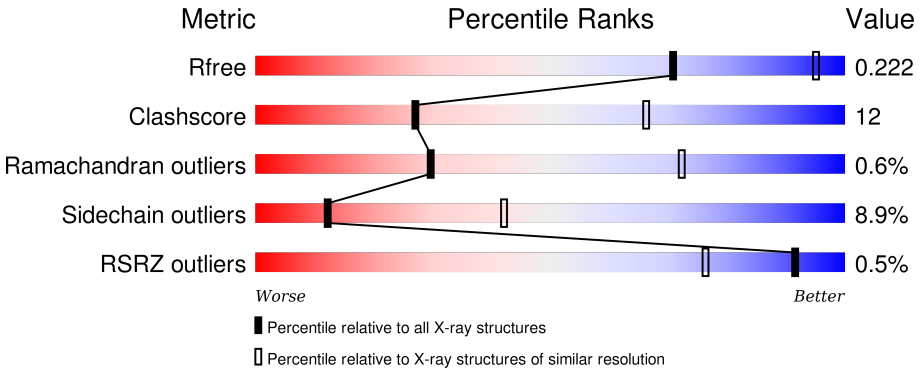
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 3.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	362	62% 28% • 7%
1	B	362	% 67% 24% • 6%
1	E	362	67% 23% • 7%
1	F	362	65% 25% • 6%
1	I	362	2% 65% 25% • 6%

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Mol	Chain	Length	Quality of chain
2	C	65	78% 14% • 6%
2	D	65	82% 11% • 6%
2	G	65	85% 9% 6%
2	H	65	83% 11% 6%
2	J	65	85% 9% 6%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	PO4	A	365	-	-	-	X
4	PO4	D	7	-	-	-	X
4	PO4	E	364	-	-	-	X
4	PO4	F	363	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 15873 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 ATPase GET3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	338	Total	C	N	O	S	0	0	0
			2643	1667	441	516	19			
1	B	341	Total	C	N	O	S	0	0	0
			2663	1678	444	522	19			
1	E	338	Total	C	N	O	S	0	0	0
			2639	1665	441	514	19			
1	F	341	Total	C	N	O	S	0	0	0
			2663	1678	444	522	19			
1	I	339	Total	C	N	O	S	0	0	0
			2647	1669	442	517	19			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	355	LEU	-	EXPRESSION TAG	UNP Q12154
A	356	GLU	-	EXPRESSION TAG	UNP Q12154
A	357	HIS	-	EXPRESSION TAG	UNP Q12154
A	358	HIS	-	EXPRESSION TAG	UNP Q12154
A	359	HIS	-	EXPRESSION TAG	UNP Q12154
A	360	HIS	-	EXPRESSION TAG	UNP Q12154
A	361	HIS	-	EXPRESSION TAG	UNP Q12154
A	362	HIS	-	EXPRESSION TAG	UNP Q12154
B	355	LEU	-	EXPRESSION TAG	UNP Q12154
B	356	GLU	-	EXPRESSION TAG	UNP Q12154
B	357	HIS	-	EXPRESSION TAG	UNP Q12154
B	358	HIS	-	EXPRESSION TAG	UNP Q12154
B	359	HIS	-	EXPRESSION TAG	UNP Q12154
B	360	HIS	-	EXPRESSION TAG	UNP Q12154
B	361	HIS	-	EXPRESSION TAG	UNP Q12154
B	362	HIS	-	EXPRESSION TAG	UNP Q12154
E	355	LEU	-	EXPRESSION TAG	UNP Q12154
E	356	GLU	-	EXPRESSION TAG	UNP Q12154
E	357	HIS	-	EXPRESSION TAG	UNP Q12154

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Chain	Residue	Modelled	Actual	Comment	Reference
E	358	HIS	-	EXPRESSION TAG	UNP Q12154
E	359	HIS	-	EXPRESSION TAG	UNP Q12154
E	360	HIS	-	EXPRESSION TAG	UNP Q12154
E	361	HIS	-	EXPRESSION TAG	UNP Q12154
E	362	HIS	-	EXPRESSION TAG	UNP Q12154
F	355	LEU	-	EXPRESSION TAG	UNP Q12154
F	356	GLU	-	EXPRESSION TAG	UNP Q12154
F	357	HIS	-	EXPRESSION TAG	UNP Q12154
F	358	HIS	-	EXPRESSION TAG	UNP Q12154
F	359	HIS	-	EXPRESSION TAG	UNP Q12154
F	360	HIS	-	EXPRESSION TAG	UNP Q12154
F	361	HIS	-	EXPRESSION TAG	UNP Q12154
F	362	HIS	-	EXPRESSION TAG	UNP Q12154
I	355	LEU	-	EXPRESSION TAG	UNP Q12154
I	356	GLU	-	EXPRESSION TAG	UNP Q12154
I	357	HIS	-	EXPRESSION TAG	UNP Q12154
I	358	HIS	-	EXPRESSION TAG	UNP Q12154
I	359	HIS	-	EXPRESSION TAG	UNP Q12154
I	360	HIS	-	EXPRESSION TAG	UNP Q12154
I	361	HIS	-	EXPRESSION TAG	UNP Q12154
I	362	HIS	-	EXPRESSION TAG	UNP Q12154

- Molecule 2 is a protein called Golgi to ER traffic protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	61	Total	C	N	O	S	0	0	0
			515	317	95	102	1			
2	D	61	Total	C	N	O	S	0	0	0
			515	317	95	102	1			
2	G	61	Total	C	N	O	S	0	0	0
			515	317	95	102	1			
2	H	61	Total	C	N	O	S	0	0	0
			515	317	95	102	1			
2	J	61	Total	C	N	O	S	0	0	0
			515	317	95	102	1			

There are 35 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	35	MET	-	EXPRESSION TAG	UNP P53192
C	94	HIS	-	EXPRESSION TAG	UNP P53192
C	95	HIS	-	EXPRESSION TAG	UNP P53192

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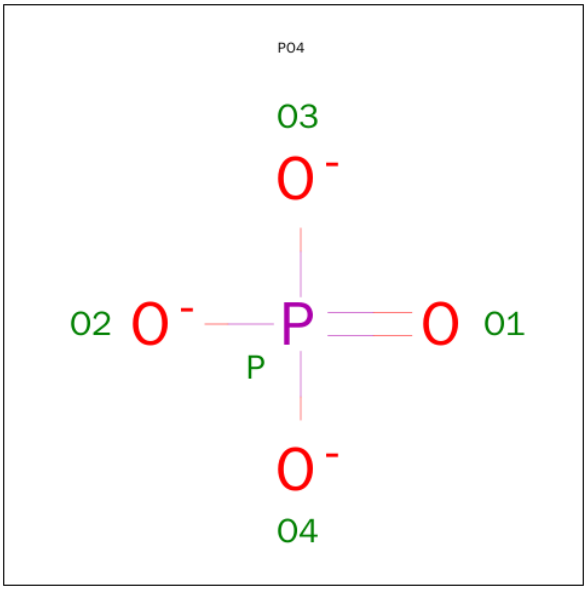
Chain	Residue	Modelled	Actual	Comment	Reference
C	96	HIS	-	EXPRESSION TAG	UNP P53192
C	97	HIS	-	EXPRESSION TAG	UNP P53192
C	98	HIS	-	EXPRESSION TAG	UNP P53192
C	99	HIS	-	EXPRESSION TAG	UNP P53192
D	35	MET	-	EXPRESSION TAG	UNP P53192
D	94	HIS	-	EXPRESSION TAG	UNP P53192
D	95	HIS	-	EXPRESSION TAG	UNP P53192
D	96	HIS	-	EXPRESSION TAG	UNP P53192
D	97	HIS	-	EXPRESSION TAG	UNP P53192
D	98	HIS	-	EXPRESSION TAG	UNP P53192
D	99	HIS	-	EXPRESSION TAG	UNP P53192
G	35	MET	-	EXPRESSION TAG	UNP P53192
G	94	HIS	-	EXPRESSION TAG	UNP P53192
G	95	HIS	-	EXPRESSION TAG	UNP P53192
G	96	HIS	-	EXPRESSION TAG	UNP P53192
G	97	HIS	-	EXPRESSION TAG	UNP P53192
G	98	HIS	-	EXPRESSION TAG	UNP P53192
G	99	HIS	-	EXPRESSION TAG	UNP P53192
H	35	MET	-	EXPRESSION TAG	UNP P53192
H	94	HIS	-	EXPRESSION TAG	UNP P53192
H	95	HIS	-	EXPRESSION TAG	UNP P53192
H	96	HIS	-	EXPRESSION TAG	UNP P53192
H	97	HIS	-	EXPRESSION TAG	UNP P53192
H	98	HIS	-	EXPRESSION TAG	UNP P53192
H	99	HIS	-	EXPRESSION TAG	UNP P53192
J	35	MET	-	EXPRESSION TAG	UNP P53192
J	94	HIS	-	EXPRESSION TAG	UNP P53192
J	95	HIS	-	EXPRESSION TAG	UNP P53192
J	96	HIS	-	EXPRESSION TAG	UNP P53192
J	97	HIS	-	EXPRESSION TAG	UNP P53192
J	98	HIS	-	EXPRESSION TAG	UNP P53192
J	99	HIS	-	EXPRESSION TAG	UNP P53192

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	I	1	Total Zn 1 1	0	0
3	A	1	Total Zn 1 1	0	0
3	E	1	Total Zn 1 1	0	0

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total O P 5 4 1	0	0
4	A	1	Total O P 5 4 1	0	0
4	B	1	Total O P 5 4 1	0	0
4	D	1	Total O P 5 4 1	0	0
4	E	1	Total O P 5 4 1	0	0
4	F	1	Total O P 5 4 1	0	0
4	I	1	Total O P 5 4 1	0	0

- Molecule 5 is water.

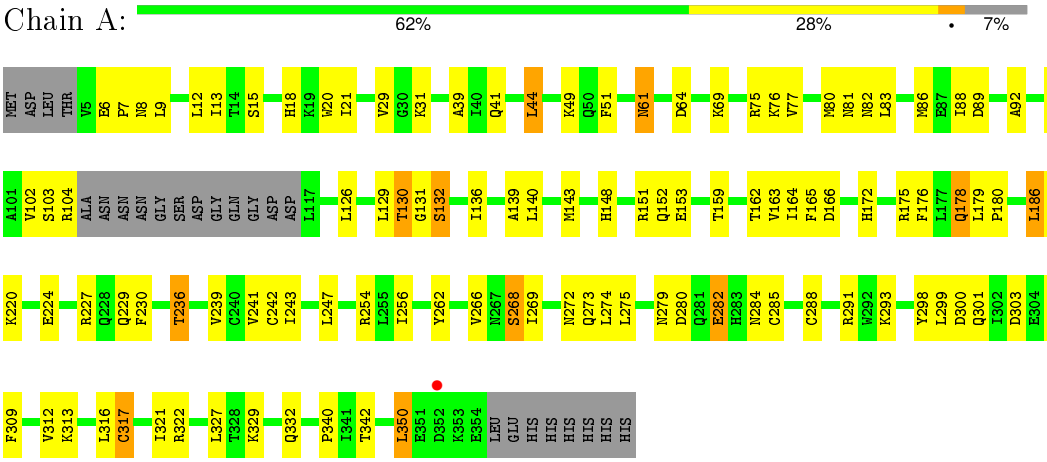
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total O 1 1	0	0
5	B	1	Total O 1 1	0	0
5	F	2	Total O 2 2	0	0
5	I	1	Total O 1 1	0	0

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.

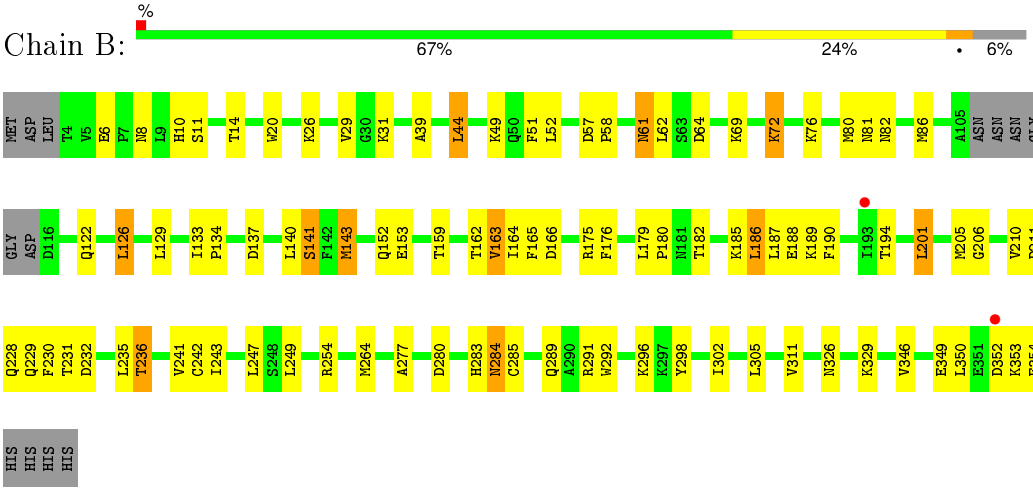
- Molecule 1: ATPase GET3

Chain A:



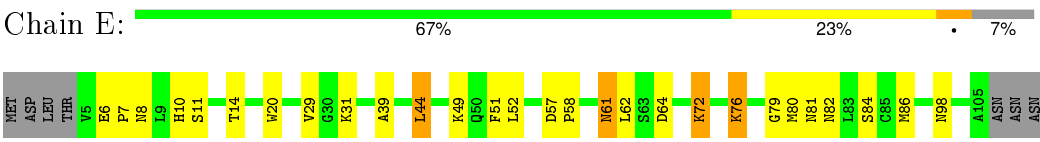
- Molecule 1: ATPase GET3

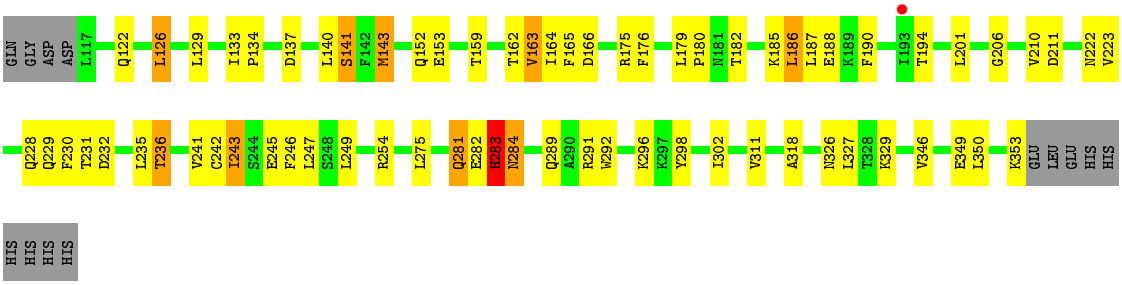
Chain B:



- Molecule 1: ATPase GET3

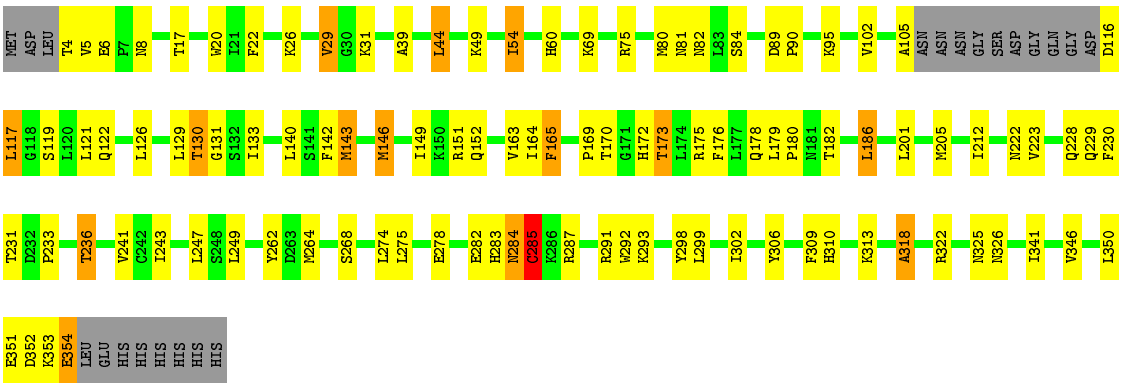
Chain E:





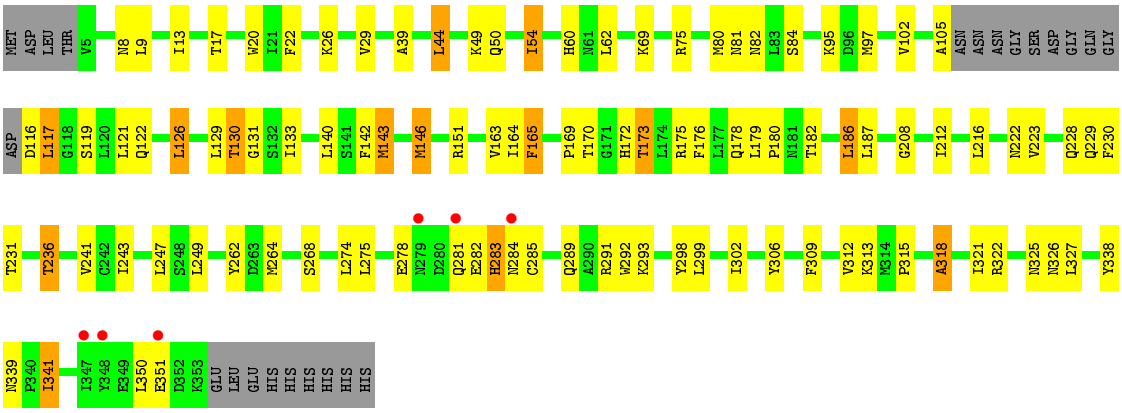
• Molecule 1: ATPase GET3

Chain F:



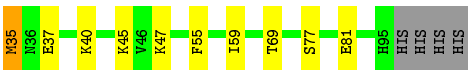
• Molecule 1: ATPase GET3

Chain I:



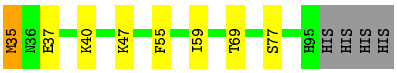
• Molecule 2: Golgi to ER traffic protein 1

Chain C:



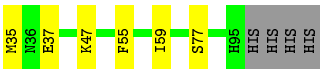
• Molecule 2: Golgi to ER traffic protein 1

Chain D:



• Molecule 2: Golgi to ER traffic protein 1

Chain G:

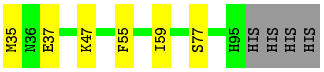


• Molecule 2: Golgi to ER traffic protein 1

Chain H:

• Molecule 2: Golgi to ER traffic protein 1

Chain J:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	204.12Å 91.46Å 149.18Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	51.30 – 3.00 51.27 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.4 (51.30-3.00) 99.5 (51.27-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$< I/\sigma(I) >$ [1]	2.52 (at 3.01Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6_289)	Depositor
R, R_{free}	0.181 , 0.231 0.172 , 0.222	Depositor DCC
R_{free} test set	2859 reflections (5.07%)	DCC
Wilson B-factor (Å^2)	76.6	Xtriage
Anisotropy	0.087	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 73.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	1 of 56410 reflections (0.002%)	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	15873	wwPDB-VP
Average B, all atoms (Å^2)	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.43% 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, 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	0.44	0/2686	0.61	0/3621
1	B	0.46	0/2706	0.60	0/3649
1	E	0.45	0/2682	0.62	0/3616
1	F	0.40	0/2706	0.56	0/3649
1	I	0.40	0/2690	0.57	0/3627
2	C	0.40	0/522	0.49	0/696
2	D	0.40	0/522	0.48	0/696
2	G	0.39	0/522	0.48	0/696
2	H	0.38	0/522	0.48	0/696
2	J	0.37	0/522	0.50	0/696
All	All	0.43	0/16080	0.58	0/21642

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	2
1	F	0	1
All	All	0	3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	26	LYS	Peptide

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Mol	Chain	Res	Type	Group
1	B	284	ASN	Peptide
1	F	284	ASN	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2643	0	2628	81	0
1	B	2663	0	2645	79	0
1	E	2639	0	2627	80	0
1	F	2663	0	2644	67	0
1	I	2647	0	2631	74	0
2	C	515	0	505	4	0
2	D	515	0	505	3	0
2	G	515	0	505	1	0
2	H	515	0	505	2	0
2	J	515	0	505	1	0
3	A	1	0	0	0	0
3	E	1	0	0	0	0
3	I	1	0	0	0	0
4	A	10	0	0	0	0
4	B	5	0	0	0	0
4	D	5	0	0	0	0
4	E	5	0	0	0	0
4	F	5	0	0	1	0
4	I	5	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	F	2	0	0	0	0
5	I	1	0	0	0	0
All	All	15873	0	15700	378	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 (378) 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:352:ASP:HB3	1:I:69:LYS:HB3	1.36	1.03
1:A:9:LEU:O	1:A:13:ILE:HG13	1.68	0.94
1:A:230:PHE:HA	1:A:236:THR:HG21	1.49	0.93
1:A:239:VAL:HG13	1:A:268:SER:HB2	1.53	0.89
1:I:281:GLN:HA	1:I:283:HIS:ND1	1.87	0.89
1:E:29:VAL:HG12	1:E:241:VAL:HG12	1.56	0.87
1:B:29:VAL:HG12	1:B:241:VAL:HG12	1.53	0.87
1:B:352:ASP:CB	1:I:69:LYS:HB3	2.04	0.87
1:B:20:TRP:HB2	1:B:236:THR:HB	1.61	0.81
1:B:31:LYS:HE3	1:B:166:ASP:OD1	1.79	0.81
1:F:230:PHE:HA	1:F:236:THR:HG21	1.62	0.81
1:E:20:TRP:HB2	1:E:236:THR:HB	1.61	0.81
1:F:20:TRP:HB2	1:F:236:THR:HB	1.62	0.81
1:E:282:GLU:HB3	1:E:284:ASN:HB2	1.61	0.80
1:A:20:TRP:HB2	1:A:236:THR:HB	1.64	0.79
1:I:20:TRP:HB2	1:I:236:THR:HB	1.63	0.79
1:B:72:LYS:HE2	1:F:282:GLU:HG3	1.65	0.77
1:A:31:LYS:HE3	1:A:166:ASP:OD1	1.84	0.76
1:I:282:GLU:HG3	1:I:284:ASN:H	1.51	0.76
1:I:230:PHE:HA	1:I:236:THR:HG21	1.68	0.76
1:E:31:LYS:HE3	1:E:166:ASP:OD1	1.85	0.76
1:E:179:LEU:N	1:E:180:PRO:HD2	2.04	0.72
1:F:179:LEU:N	1:F:180:PRO:HD2	2.07	0.70
1:B:230:PHE:HA	1:B:236:THR:HG21	1.72	0.70
1:E:349:GLU:O	1:E:353:LYS:HG2	1.93	0.69
1:F:299:LEU:HD22	1:F:313:LYS:HE3	1.75	0.69
1:E:72:LYS:CD	1:E:72:LYS:H	2.05	0.69
1:F:180:PRO:HD3	1:F:223:VAL:HG11	1.72	0.68
1:A:39:ALA:HA	1:A:164:ILE:CD1	2.24	0.68
1:E:282:GLU:C	1:E:284:ASN:N	2.43	0.68
1:B:349:GLU:O	1:B:353:LYS:HG2	1.93	0.68
1:I:180:PRO:HD3	1:I:223:VAL:HG11	1.75	0.68
1:A:285:CYS:HB3	1:A:288:CYS:HB2	1.76	0.67
1:F:29:VAL:HG13	1:F:241:VAL:HG12	1.76	0.67
1:A:172:HIS:HB2	1:A:175:ARG:HH11	1.57	0.67
1:B:29:VAL:CG1	1:B:241:VAL:HG12	2.25	0.67
1:B:179:LEU:N	1:B:180:PRO:HD2	2.09	0.66
1:E:52:LEU:HD11	1:E:86:MET:HG2	1.77	0.66
1:B:180:PRO:HD3	1:B:223:VAL:HG11	1.78	0.66
1:E:29:VAL:CG1	1:E:241:VAL:HG12	2.25	0.65
1:B:72:LYS:H	1:B:72:LYS:CD	2.07	0.65
1:E:254:ARG:HH11	1:E:254:ARG:HB3	1.62	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:136:ILE:HD13	1:A:179:LEU:HD21	1.78	0.64
1:E:72:LYS:H	1:E:72:LYS:HD2	1.62	0.63
1:A:29:VAL:HG12	1:A:241:VAL:HG12	1.79	0.63
1:I:179:LEU:N	1:I:180:PRO:HD2	2.13	0.63
1:I:299:LEU:HD22	1:I:313:LYS:HE3	1.80	0.63
1:F:228:GLN:HE21	1:F:229:GLN:HG2	1.62	0.63
1:E:329:LYS:HD3	1:E:350:LEU:HD11	1.80	0.63
1:B:232:ASP:HB3	1:B:235:LEU:HB2	1.79	0.62
1:E:230:PHE:HA	1:E:236:THR:HG21	1.80	0.62
1:I:29:VAL:HG13	1:I:241:VAL:HG12	1.80	0.62
1:B:72:LYS:H	1:B:72:LYS:HD2	1.65	0.62
1:B:86:MET:HE1	1:B:152:GLN:HG3	1.81	0.62
1:F:176:PHE:O	1:F:179:LEU:HB2	1.99	0.62
1:E:229:GLN:O	1:E:236:THR:HG23	2.00	0.62
1:B:254:ARG:HH11	1:B:254:ARG:HB3	1.65	0.62
1:F:22:PHE:CE1	1:F:165:PHE:HD1	2.17	0.61
1:E:44:LEU:HD13	1:E:80:MET:HE1	1.81	0.61
1:E:180:PRO:HD3	1:E:223:VAL:HG11	1.82	0.61
1:F:354:GLU:HG2	1:F:354:GLU:O	2.00	0.61
1:B:52:LEU:HD11	1:B:86:MET:HG2	1.82	0.61
1:E:232:ASP:HB3	1:E:235:LEU:HB2	1.81	0.61
1:I:228:GLN:HE21	1:I:229:GLN:HG2	1.65	0.60
1:A:178:GLN:C	1:A:180:PRO:HD2	2.22	0.60
1:I:176:PHE:O	1:I:179:LEU:HB2	2.02	0.59
1:F:22:PHE:CE1	1:F:165:PHE:CD1	2.90	0.59
1:E:39:ALA:HA	1:E:164:ILE:CD1	2.31	0.59
1:B:39:ALA:HA	1:B:164:ILE:CD1	2.32	0.59
1:I:22:PHE:CE1	1:I:165:PHE:CD1	2.90	0.59
1:I:143:MET:SD	1:I:222:ASN:HB3	2.43	0.59
1:B:44:LEU:HD13	1:B:80:MET:HE1	1.84	0.58
1:B:329:LYS:HD3	1:B:350:LEU:HD11	1.85	0.58
1:F:143:MET:SD	1:F:222:ASN:HB3	2.43	0.58
1:I:22:PHE:CE1	1:I:165:PHE:HD1	2.21	0.58
1:F:26:LYS:HG3	1:F:169:PRO:O	2.04	0.58
1:A:95:LYS:HE2	1:A:99:ASP:OD2	2.04	0.58
1:E:86:MET:HE1	1:E:152:GLN:HG3	1.84	0.58
1:F:29:VAL:HG22	1:F:243:ILE:HG23	1.86	0.58
1:A:29:VAL:HG11	1:A:242:CYS:CA	2.33	0.58
1:B:185:LYS:O	1:B:188:GLU:HG2	2.03	0.58
1:I:69:LYS:O	1:I:75:ARG:NH2	2.37	0.58
1:I:26:LYS:HG3	1:I:169:PRO:O	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:230:PHE:HA	1:I:236:THR:CG2	2.35	0.57
1:B:143:MET:CE	1:B:222:ASN:HB3	2.34	0.57
1:I:298:TYR:O	1:I:302:ILE:HG13	2.04	0.57
1:E:185:LYS:O	1:E:188:GLU:HG2	2.05	0.57
1:B:229:GLN:O	1:B:236:THR:HG23	2.05	0.57
1:A:29:VAL:HG12	1:A:29:VAL:O	2.05	0.57
1:F:49:LYS:O	1:F:82:ASN:HB2	2.04	0.57
1:F:230:PHE:HA	1:F:236:THR:CG2	2.33	0.56
1:E:176:PHE:O	1:E:179:LEU:HB2	2.05	0.56
1:E:179:LEU:N	1:E:180:PRO:CD	2.67	0.56
1:B:20:TRP:CE3	1:B:163:VAL:HG22	2.41	0.56
1:A:180:PRO:HG3	1:A:227:ARG:NH1	2.21	0.56
1:E:61:ASN:H	1:E:61:ASN:ND2	2.03	0.56
1:E:20:TRP:CE3	1:E:163:VAL:HG22	2.41	0.56
1:B:61:ASN:ND2	1:B:61:ASN:H	2.03	0.56
1:E:143:MET:CE	1:E:222:ASN:HB3	2.36	0.56
1:I:49:LYS:O	1:I:82:ASN:HB2	2.06	0.56
1:E:318:ALA:HB2	1:F:287:ARG:HG2	1.87	0.56
1:B:352:ASP:HB2	1:I:75:ARG:HH22	1.70	0.56
1:I:322:ARG:O	1:I:326:ASN:HB2	2.06	0.56
1:B:229:GLN:O	1:B:236:THR:CG2	2.54	0.55
1:B:69:LYS:CB	1:F:352:ASP:HB3	2.36	0.55
1:B:69:LYS:HB2	1:F:352:ASP:HB3	1.88	0.55
1:B:176:PHE:O	1:B:179:LEU:HB2	2.06	0.55
1:I:231:THR:HG22	1:I:231:THR:O	2.05	0.55
1:A:220:LYS:HG2	1:A:224:GLU:OE1	2.06	0.55
1:B:72:LYS:CE	1:F:282:GLU:HG3	2.36	0.55
1:I:105:ALA:HB1	1:I:119:SER:OG	2.06	0.55
1:B:179:LEU:N	1:B:180:PRO:CD	2.70	0.55
1:B:352:ASP:CG	1:I:69:LYS:HB3	2.27	0.55
1:B:277:ALA:HA	1:B:284:ASN:ND2	2.21	0.55
1:E:228:GLN:NE2	1:E:229:GLN:HG2	2.22	0.55
1:A:29:VAL:HG11	1:A:242:CYS:HA	1.90	0.55
1:F:105:ALA:HB1	1:F:119:SER:OG	2.07	0.55
1:I:350:LEU:H	1:I:350:LEU:HD12	1.72	0.55
1:I:29:VAL:HG22	1:I:243:ILE:HG23	1.90	0.54
1:F:130:THR:HG22	1:F:131:GLY:N	2.21	0.54
1:A:12:LEU:HD11	1:A:21:ILE:HD13	1.88	0.54
1:B:228:GLN:NE2	1:B:229:GLN:HG2	2.23	0.54
1:B:10:HIS:O	1:B:14:THR:HG23	2.07	0.54
1:E:10:HIS:O	1:E:14:THR:HG23	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:280:ASP:OD2	1:B:283:HIS:HB2	2.08	0.54
1:E:190:PHE:O	1:E:194:THR:HG23	2.08	0.54
1:F:322:ARG:O	1:F:326:ASN:HB2	2.08	0.53
1:I:229:GLN:O	1:I:236:THR:CG2	2.56	0.53
1:I:180:PRO:HD3	1:I:223:VAL:CG1	2.37	0.53
1:I:274:LEU:CD1	1:I:313:LYS:HB3	2.39	0.53
1:A:49:LYS:O	1:A:82:ASN:HB2	2.08	0.53
1:F:231:THR:O	1:F:231:THR:HG22	2.07	0.53
1:A:282:GLU:C	1:A:284:ASN:N	2.62	0.53
1:A:77:VAL:HG23	1:A:83:LEU:O	2.10	0.52
1:E:29:VAL:HG12	1:E:29:VAL:O	2.10	0.52
1:I:249:LEU:HD11	1:I:298:TYR:HB3	1.90	0.52
1:B:137:ASP:O	1:B:141:SER:HB2	2.10	0.52
1:F:180:PRO:HD3	1:F:223:VAL:CG1	2.38	0.52
1:I:282:GLU:C	1:I:284:ASN:N	2.62	0.52
1:I:142:PHE:CZ	1:I:146:MET:HE1	2.45	0.52
1:F:274:LEU:CD1	1:F:313:LYS:HB3	2.39	0.52
2:H:55:PHE:CE2	2:H:59:ILE:HD11	2.44	0.52
1:F:249:LEU:HD11	1:F:298:TYR:HB3	1.92	0.52
1:A:61:ASN:H	1:A:61:ASN:ND2	2.08	0.52
1:B:277:ALA:HA	1:B:284:ASN:HD22	1.75	0.51
1:E:137:ASP:O	1:E:141:SER:HB2	2.10	0.51
1:A:275:LEU:CD2	1:A:316:LEU:HD23	2.40	0.51
1:E:61:ASN:H	1:E:61:ASN:HD22	1.57	0.51
1:B:61:ASN:H	1:B:61:ASN:HD22	1.57	0.51
1:A:275:LEU:HD23	1:A:316:LEU:HD23	1.91	0.51
1:B:175:ARG:O	1:B:175:ARG:HG3	2.10	0.51
1:F:229:GLN:O	1:F:236:THR:CG2	2.58	0.51
1:F:133:ILE:HD11	1:F:186:LEU:HD13	1.92	0.51
1:F:130:THR:CG2	1:F:131:GLY:N	2.74	0.51
1:I:130:THR:HG22	1:I:131:GLY:N	2.24	0.51
2:C:55:PHE:CE2	2:C:59:ILE:HD11	2.46	0.51
1:B:29:VAL:HG11	1:B:242:CYS:HA	1.92	0.50
1:A:272:ASN:HB3	1:A:273:GLN:HG3	1.94	0.50
1:F:69:LYS:O	1:F:75:ARG:NH2	2.44	0.50
1:A:153:GLU:HG2	1:A:159:THR:HA	1.93	0.50
1:F:39:ALA:HA	1:F:164:ILE:CD1	2.42	0.50
1:A:329:LYS:O	1:A:332:GLN:HG2	2.12	0.50
1:E:229:GLN:O	1:E:236:THR:CG2	2.60	0.50
1:F:179:LEU:N	1:F:180:PRO:CD	2.73	0.50
2:D:55:PHE:CE2	2:D:59:ILE:HD11	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:55:PHE:CE2	2:J:59:ILE:HD11	2.47	0.50
1:I:282:GLU:O	1:I:283:HIS:C	2.49	0.50
1:I:39:ALA:HA	1:I:164:ILE:CD1	2.41	0.50
1:I:44:LEU:HD13	1:I:80:MET:HE1	1.94	0.49
1:B:190:PHE:O	1:B:194:THR:HG23	2.11	0.49
1:B:326:ASN:ND2	1:B:326:ASN:H	2.10	0.49
1:I:282:GLU:HG3	1:I:284:ASN:N	2.24	0.49
1:A:266:VAL:O	1:A:266:VAL:HG13	2.12	0.49
1:I:54:ILE:HG23	1:I:165:PHE:CD2	2.48	0.49
1:B:206:GLY:O	1:B:210:VAL:HG23	2.13	0.49
1:F:179:LEU:H	1:F:180:PRO:HD2	1.77	0.49
1:A:176:PHE:O	1:A:179:LEU:HB2	2.13	0.49
1:B:133:ILE:HD11	1:B:186:LEU:HD13	1.94	0.49
1:I:325:ASN:OD1	1:I:326:ASN:N	2.46	0.49
1:F:325:ASN:OD1	1:F:326:ASN:N	2.46	0.49
1:E:20:TRP:CZ3	1:E:163:VAL:HG21	2.48	0.49
1:A:129:LEU:HD23	1:A:216:LEU:HD11	1.94	0.49
1:B:49:LYS:O	1:B:82:ASN:HB2	2.13	0.49
1:F:178:GLN:NE2	1:F:262:TYR:CD1	2.81	0.49
1:A:139:ALA:O	1:A:143:MET:HG2	2.12	0.48
1:E:79:GLY:O	1:E:80:MET:HG2	2.13	0.48
2:G:55:PHE:CE2	2:G:59:ILE:HD11	2.48	0.48
1:E:281:GLN:C	1:E:283:HIS:N	2.64	0.48
1:A:9:LEU:HG	1:A:312:VAL:HG21	1.94	0.48
1:F:284:ASN:O	1:F:285:CYS:O	2.31	0.48
1:I:282:GLU:HG3	1:I:284:ASN:HB2	1.95	0.48
1:E:282:GLU:O	1:E:284:ASN:N	2.46	0.48
1:A:139:ALA:HB2	1:A:176:PHE:HB2	1.95	0.48
1:E:49:LYS:O	1:E:82:ASN:HB2	2.13	0.48
1:E:134:PRO:HB2	1:E:175:ARG:HH21	1.78	0.48
1:E:29:VAL:O	1:E:29:VAL:CG1	2.62	0.48
1:A:298:TYR:O	1:A:301:GLN:HB2	2.13	0.48
1:I:278:GLU:OE1	1:I:292:TRP:NE1	2.47	0.48
1:I:231:THR:O	1:I:231:THR:CG2	2.62	0.48
1:F:293:LYS:HA	1:F:293:LYS:HD3	1.69	0.48
1:F:117:LEU:HD22	1:F:121:LEU:HG	1.96	0.48
1:A:15:SER:OG	1:A:18:HIS:HD2	1.97	0.48
1:E:175:ARG:O	1:E:175:ARG:HG3	2.13	0.47
1:F:142:PHE:CZ	1:F:146:MET:HE1	2.49	0.47
1:A:13:ILE:HD13	1:A:41:GLN:HB3	1.97	0.47
1:E:29:VAL:HG11	1:E:242:CYS:HA	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:254:ARG:HB3	1:E:254:ARG:NH1	2.28	0.47
1:A:229:GLN:O	1:A:236:THR:CG2	2.62	0.47
1:A:29:VAL:CG1	1:A:241:VAL:HG12	2.45	0.47
1:F:143:MET:HB3	1:F:143:MET:HE3	1.48	0.47
1:I:130:THR:CG2	1:I:131:GLY:N	2.77	0.47
1:B:6:GLU:HB3	1:B:8:ASN:ND2	2.30	0.47
1:A:86:MET:HE3	1:A:152:GLN:HG3	1.95	0.47
1:F:298:TYR:O	1:F:302:ILE:HG13	2.14	0.47
1:F:6:GLU:HB3	1:F:8:ASN:ND2	2.29	0.47
1:B:187:LEU:HA	1:B:187:LEU:HD23	1.74	0.47
1:I:282:GLU:O	1:I:284:ASN:N	2.47	0.47
1:E:346:VAL:O	1:E:350:LEU:HD13	2.14	0.47
1:E:187:LEU:HA	1:E:187:LEU:HD23	1.79	0.47
1:I:281:GLN:C	1:I:283:HIS:N	2.63	0.47
1:F:54:ILE:HG23	1:F:165:PHE:CD2	2.50	0.47
1:E:61:ASN:ND2	1:E:61:ASN:N	2.62	0.47
1:B:29:VAL:O	1:B:29:VAL:HG12	2.14	0.47
1:F:149:ILE:O	1:F:152:GLN:HB2	2.15	0.47
1:A:20:TRP:O	1:A:236:THR:HA	2.16	0.46
1:I:179:LEU:N	1:I:180:PRO:CD	2.78	0.46
1:I:178:GLN:NE2	1:I:262:TYR:CD1	2.84	0.46
1:F:306:TYR:HB3	1:F:309:PHE:HB2	1.96	0.46
1:E:133:ILE:HD11	1:E:186:LEU:HD13	1.96	0.46
1:E:62:LEU:HD23	1:E:62:LEU:HA	1.65	0.46
1:A:69:LYS:HD2	1:A:69:LYS:N	2.30	0.46
1:B:153:GLU:HG2	1:B:159:THR:HA	1.97	0.46
1:E:281:GLN:O	1:E:282:GLU:C	2.53	0.46
1:F:231:THR:O	1:F:231:THR:CG2	2.63	0.46
1:B:231:THR:O	1:B:231:THR:CG2	2.63	0.46
1:I:133:ILE:HD11	1:I:186:LEU:HD13	1.97	0.46
1:B:29:VAL:HG11	1:B:242:CYS:CA	2.46	0.46
1:E:282:GLU:O	1:E:283:HIS:C	2.54	0.46
1:A:178:GLN:NE2	1:A:262:TYR:CD1	2.84	0.46
1:E:326:ASN:H	1:E:326:ASN:ND2	2.14	0.46
1:B:134:PRO:HB2	1:B:175:ARG:HH21	1.81	0.46
1:A:279:ASN:CB	1:A:340:PRO:HB2	2.46	0.46
1:I:143:MET:HB3	1:I:143:MET:HE3	1.44	0.45
1:B:298:TYR:O	1:B:302:ILE:HG13	2.16	0.45
1:E:153:GLU:HG2	1:E:159:THR:HA	1.98	0.45
1:B:62:LEU:HD23	1:B:62:LEU:HA	1.60	0.45
1:B:254:ARG:NH1	1:B:254:ARG:HB3	2.29	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:29:VAL:HG13	1:A:243:ILE:HG23	1.97	0.45
1:A:282:GLU:C	1:A:284:ASN:H	2.19	0.45
1:A:316:LEU:HD12	1:A:317:CYS:N	2.30	0.45
1:F:275:LEU:HA	1:F:275:LEU:HD23	1.62	0.45
1:A:282:GLU:O	1:A:284:ASN:N	2.50	0.45
1:F:44:LEU:HD13	1:F:80:MET:HE1	1.98	0.45
1:A:299:LEU:HD23	1:A:299:LEU:HA	1.66	0.45
1:B:235:LEU:HA	1:B:235:LEU:HD23	1.69	0.45
1:E:51:PHE:HD1	1:E:162:THR:HB	1.82	0.45
1:I:117:LEU:HD22	1:I:121:LEU:HG	1.99	0.45
1:A:61:ASN:N	1:A:61:ASN:ND2	2.64	0.45
1:F:278:GLU:OE1	1:F:292:TRP:NE1	2.50	0.45
1:E:235:LEU:HD23	1:E:235:LEU:HA	1.75	0.45
1:E:249:LEU:HD11	1:E:298:TYR:HB3	1.99	0.45
1:A:8:ASN:HA	1:A:312:VAL:HG13	1.98	0.45
1:A:329:LYS:HE2	1:A:329:LYS:HB3	1.75	0.45
1:B:126:LEU:HA	1:B:126:LEU:HD13	1.86	0.45
1:E:292:TRP:CZ2	1:E:296:LYS:HE3	2.52	0.45
1:E:230:PHE:HA	1:E:236:THR:CG2	2.46	0.44
1:F:122:GLN:HE22	1:F:212:ILE:HG13	1.81	0.44
1:A:230:PHE:CA	1:A:236:THR:HG21	2.33	0.44
1:A:187:LEU:HA	1:A:187:LEU:HD23	1.79	0.44
1:B:57:ASP:HA	1:B:58:PRO:HD3	1.84	0.44
1:A:256:ILE:HD13	1:A:309:PHE:HE2	1.81	0.44
1:B:352:ASP:CG	1:I:69:LYS:HG2	2.37	0.44
1:A:280:ASP:OD1	1:A:282:GLU:HG2	2.17	0.44
1:A:256:ILE:HD13	1:A:309:PHE:CE2	2.52	0.44
1:B:292:TRP:CZ2	1:B:296:LYS:HE3	2.52	0.44
1:B:201:LEU:HD12	1:B:201:LEU:HA	1.87	0.44
1:E:275:LEU:HA	1:E:275:LEU:HD23	1.82	0.44
1:E:122:GLN:HE22	1:E:211:ASP:HB3	1.83	0.44
1:I:293:LYS:HD3	1:I:293:LYS:HA	1.70	0.44
1:A:130:THR:C	1:A:132:SER:H	2.21	0.44
1:F:172:HIS:O	1:F:173:THR:C	2.55	0.44
1:F:178:GLN:NE2	1:F:262:TYR:HD1	2.15	0.44
1:F:353:LYS:O	1:F:354:GLU:C	2.56	0.44
1:B:122:GLN:HE22	1:B:211:ASP:HB3	1.83	0.44
1:F:353:LYS:HE2	1:F:353:LYS:HB2	1.74	0.43
1:E:6:GLU:HB3	1:E:8:ASN:ND2	2.33	0.43
1:A:179:LEU:N	1:A:180:PRO:HD2	2.33	0.43
1:A:6:GLU:HA	1:A:7:PRO:HD2	1.70	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:350:LEU:HA	1:A:350:LEU:HD12	1.83	0.43
1:A:148:HIS:HA	1:A:151:ARG:HE	1.82	0.43
1:B:230:PHE:HA	1:B:236:THR:CG2	2.43	0.43
1:E:20:TRP:CE3	1:E:163:VAL:CG2	3.01	0.43
1:E:51:PHE:CD1	1:E:162:THR:HB	2.53	0.43
1:A:179:LEU:N	1:A:180:PRO:CD	2.81	0.43
1:B:86:MET:CE	1:B:152:GLN:HG3	2.48	0.43
1:B:305:LEU:HD21	2:C:69:THR:HG21	2.00	0.43
1:F:89:ASP:HA	1:F:90:PRO:HD3	1.87	0.43
1:B:29:VAL:O	1:B:29:VAL:CG1	2.66	0.43
1:I:178:GLN:NE2	1:I:262:TYR:HD1	2.17	0.43
1:A:186:LEU:HD23	1:A:187:LEU:N	2.32	0.43
1:A:100:MET:HB3	1:A:104:ARG:HH21	1.83	0.43
1:I:9:LEU:O	1:I:13:ILE:HG13	2.18	0.43
1:B:20:TRP:CZ3	1:B:163:VAL:HG21	2.54	0.43
1:A:89:ASP:HB3	1:A:92:ALA:HB3	2.00	0.43
1:E:98:ASN:N	1:E:98:ASN:HD22	2.17	0.43
1:E:243:ILE:HG13	1:E:245:GLU:HG3	2.01	0.43
1:E:249:LEU:HD21	1:E:302:ILE:HD11	2.01	0.43
1:F:346:VAL:O	1:F:350:LEU:CD1	2.67	0.43
1:A:300:ASP:O	1:A:303:ASP:HB2	2.19	0.43
1:E:206:GLY:O	1:E:210:VAL:HG23	2.19	0.42
1:B:352:ASP:CB	1:I:75:ARG:HH22	2.32	0.42
1:A:29:VAL:HG11	1:A:242:CYS:N	2.34	0.42
1:A:269:ILE:HG13	1:A:309:PHE:HD2	1.83	0.42
1:B:354:GLU:CD	1:B:354:GLU:C	2.78	0.42
1:A:280:ASP:CG	1:A:282:GLU:HG2	2.38	0.42
1:B:20:TRP:O	1:B:236:THR:HA	2.19	0.42
1:F:31:LYS:HB3	4:F:363:PO4:O1	2.20	0.42
1:A:293:LYS:HA	1:A:293:LYS:HD3	1.59	0.42
1:E:143:MET:HE2	1:E:222:ASN:HB3	2.00	0.42
1:I:350:LEU:HD12	1:I:350:LEU:N	2.35	0.42
1:A:86:MET:CE	1:A:152:GLN:HG3	2.50	0.42
1:A:44:LEU:HD12	1:A:44:LEU:HA	1.80	0.42
2:C:35:MET:HE3	2:C:40:LYS:HG2	2.01	0.42
1:I:299:LEU:HD23	1:I:299:LEU:HA	1.83	0.42
1:A:15:SER:OG	1:A:18:HIS:CD2	2.72	0.42
2:C:45:LYS:HE3	2:C:81:GLU:OE1	2.19	0.42
1:A:51:PHE:CD1	1:A:162:THR:HB	2.55	0.42
1:E:231:THR:O	1:E:231:THR:CG2	2.67	0.42
1:I:172:HIS:O	1:I:173:THR:C	2.58	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:62:LEU:HA	1:I:62:LEU:HD23	1.78	0.42
1:I:8:ASN:HA	1:I:312:VAL:HG22	2.02	0.42
1:E:31:LYS:HB3	1:E:31:LYS:HE2	1.66	0.41
1:A:88:ILE:HG12	1:A:89:ASP:N	2.34	0.41
1:F:350:LEU:HD12	1:F:350:LEU:H	1.85	0.41
1:B:346:VAL:O	1:B:350:LEU:HD13	2.21	0.41
1:I:126:LEU:O	1:I:130:THR:HB	2.21	0.41
1:I:187:LEU:HD21	1:I:216:LEU:HB2	2.03	0.41
1:I:97:MET:HE2	1:I:97:MET:HB3	1.89	0.41
1:I:315:PRO:HB3	1:I:338:TYR:CE2	2.55	0.41
1:E:29:VAL:HG22	1:E:243:ILE:HG23	2.01	0.41
1:B:51:PHE:HD1	1:B:162:THR:HB	1.85	0.41
1:A:305:LEU:HD21	2:D:69:THR:HG21	2.02	0.41
1:E:61:ASN:HD22	1:E:61:ASN:N	2.16	0.41
1:I:208:GLY:O	1:I:212:ILE:HG13	2.20	0.41
1:E:57:ASP:HA	1:E:58:PRO:HD3	1.83	0.41
1:I:321:ILE:HG22	1:I:327:LEU:HD23	2.02	0.41
1:E:76:LYS:HD2	1:E:84:SER:OG	2.21	0.41
1:E:126:LEU:HA	1:E:126:LEU:HD13	1.85	0.41
1:E:245:GLU:O	1:E:246:PHE:C	2.59	0.41
2:H:45:LYS:HE3	2:H:81:GLU:OE1	2.20	0.41
1:B:326:ASN:HD22	1:B:326:ASN:H	1.69	0.41
1:E:6:GLU:HA	1:E:7:PRO:HD2	1.85	0.41
1:B:189:LYS:HD3	1:B:189:LYS:HA	1.84	0.41
1:I:306:TYR:HB3	1:I:309:PHE:HB2	2.03	0.41
1:E:29:VAL:HG11	1:E:242:CYS:CA	2.51	0.41
1:A:180:PRO:CG	1:A:227:ARG:NH1	2.84	0.41
1:I:318:ALA:HB3	1:I:351:GLU:HG3	2.02	0.41
1:I:50:GLN:NE2	1:I:82:ASN:HA	2.35	0.41
1:F:231:THR:O	1:F:233:PRO:HD3	2.21	0.41
1:B:249:LEU:HD11	1:B:298:TYR:HB3	2.02	0.41
1:E:298:TYR:O	1:E:302:ILE:HG13	2.20	0.41
1:I:339:ASN:OD1	1:I:341:ILE:HG13	2.20	0.41
1:A:321:ILE:HG22	1:A:327:LEU:HD23	2.03	0.41
1:A:321:ILE:CG2	1:A:327:LEU:HD23	2.50	0.41
1:F:318:ALA:HB3	1:F:351:GLU:HG3	2.02	0.41
2:D:35:MET:HE3	2:D:40:LYS:HG2	2.03	0.41
1:B:69:LYS:HB3	1:F:352:ASP:HB3	2.02	0.41
1:F:122:GLN:NE2	1:F:212:ILE:CG1	2.84	0.41
1:A:130:THR:HG22	1:A:131:GLY:N	2.36	0.41
1:E:327:LEU:HD23	1:E:327:LEU:HA	1.87	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:122:GLN:HE22	1:I:212:ILE:HG13	1.85	0.40
1:F:201:LEU:O	1:F:205:MET:HB2	2.21	0.40
1:A:274:LEU:CD1	1:A:313:LYS:HB3	2.51	0.40
1:F:282:GLU:C	1:F:284:ASN:H	2.25	0.40
1:B:61:ASN:HD22	1:B:61:ASN:N	2.16	0.40
1:F:5:VAL:HG13	1:F:310:HIS:CE1	2.57	0.40
1:I:122:GLN:NE2	1:I:212:ILE:CG1	2.84	0.40
1:I:275:LEU:HA	1:I:275:LEU:HD23	1.66	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	334/362 (92%)	317 (95%)	16 (5%)	1 (0%)	46	84
1	B	337/362 (93%)	322 (96%)	14 (4%)	1 (0%)	46	84
1	E	334/362 (92%)	321 (96%)	10 (3%)	3 (1%)	21	64
1	F	337/362 (93%)	321 (95%)	12 (4%)	4 (1%)	16	56
1	I	335/362 (92%)	318 (95%)	14 (4%)	3 (1%)	21	64
2	C	59/65 (91%)	56 (95%)	3 (5%)	0	100	100
2	D	59/65 (91%)	57 (97%)	2 (3%)	0	100	100
2	G	59/65 (91%)	57 (97%)	2 (3%)	0	100	100
2	H	59/65 (91%)	58 (98%)	1 (2%)	0	100	100
2	J	59/65 (91%)	56 (95%)	3 (5%)	0	100	100
All	All	1972/2135 (92%)	1883 (96%)	77 (4%)	12 (1%)	30	72

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	285	CYS
1	F	173	THR
1	F	285	CYS
1	F	318	ALA
1	I	173	THR
1	I	318	ALA
1	E	281	GLN
1	E	283	HIS
1	E	284	ASN
1	I	283	HIS
1	A	102	VAL
1	F	283	HIS

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	297/317 (94%)	270 (91%)	27 (9%)	12	41
1	B	299/317 (94%)	274 (92%)	25 (8%)	14	45
1	E	296/317 (93%)	272 (92%)	24 (8%)	15	47
1	F	299/317 (94%)	266 (89%)	33 (11%)	8	30
1	I	297/317 (94%)	266 (90%)	31 (10%)	9	32
2	C	58/62 (94%)	54 (93%)	4 (7%)	19	56
2	D	58/62 (94%)	54 (93%)	4 (7%)	19	56
2	G	58/62 (94%)	54 (93%)	4 (7%)	19	56
2	H	58/62 (94%)	55 (95%)	3 (5%)	29	68
2	J	58/62 (94%)	54 (93%)	4 (7%)	19	56
All	All	1778/1895 (94%)	1619 (91%)	159 (9%)	12	42

All (159) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	44	LEU
1	A	61	ASN

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Mol	Chain	Res	Type
1	A	64	ASP
1	A	75	ARG
1	A	76	LYS
1	A	80	MET
1	A	81	ASN
1	A	103	SER
1	A	126	LEU
1	A	130	THR
1	A	132	SER
1	A	140	LEU
1	A	163	VAL
1	A	165	PHE
1	A	178	GLN
1	A	186	LEU
1	A	236	THR
1	A	247	LEU
1	A	254	ARG
1	A	268	SER
1	A	282	GLU
1	A	291	ARG
1	A	307	GLU
1	A	317	CYS
1	A	322	ARG
1	A	342	THR
1	A	350	LEU
1	B	11	SER
1	B	44	LEU
1	B	61	ASN
1	B	64	ASP
1	B	72	LYS
1	B	76	LYS
1	B	81	ASN
1	B	126	LEU
1	B	129	LEU
1	B	140	LEU
1	B	141	SER
1	B	143	MET
1	B	163	VAL
1	B	165	PHE
1	B	182	THR
1	B	186	LEU
1	B	201	LEU

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Mol	Chain	Res	Type
1	B	205	MET
1	B	236	THR
1	B	243	ILE
1	B	247	LEU
1	B	264	MET
1	B	289	GLN
1	B	291	ARG
1	B	311	VAL
2	C	35	MET
2	C	37	GLU
2	C	47	LYS
2	C	77	SER
2	D	35	MET
2	D	37	GLU
2	D	47	LYS
2	D	77	SER
1	E	11	SER
1	E	44	LEU
1	E	61	ASN
1	E	64	ASP
1	E	72	LYS
1	E	76	LYS
1	E	81	ASN
1	E	126	LEU
1	E	129	LEU
1	E	140	LEU
1	E	141	SER
1	E	143	MET
1	E	163	VAL
1	E	165	PHE
1	E	182	THR
1	E	186	LEU
1	E	201	LEU
1	E	236	THR
1	E	243	ILE
1	E	247	LEU
1	E	283	HIS
1	E	289	GLN
1	E	291	ARG
1	E	311	VAL
1	F	4	THR
1	F	17	THR

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Mol	Chain	Res	Type
1	F	29	VAL
1	F	44	LEU
1	F	54	ILE
1	F	60	HIS
1	F	81	ASN
1	F	84	SER
1	F	95	LYS
1	F	102	VAL
1	F	116	ASP
1	F	117	LEU
1	F	126	LEU
1	F	129	LEU
1	F	130	THR
1	F	140	LEU
1	F	143	MET
1	F	146	MET
1	F	151	ARG
1	F	163	VAL
1	F	165	PHE
1	F	170	THR
1	F	175	ARG
1	F	182	THR
1	F	186	LEU
1	F	236	THR
1	F	247	LEU
1	F	264	MET
1	F	268	SER
1	F	285	CYS
1	F	291	ARG
1	F	341	ILE
1	F	354	GLU
2	G	35	MET
2	G	37	GLU
2	G	47	LYS
2	G	77	SER
2	H	35	MET
2	H	37	GLU
2	H	77	SER
1	I	17	THR
1	I	44	LEU
1	I	54	ILE
1	I	60	HIS

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Mol	Chain	Res	Type
1	I	81	ASN
1	I	84	SER
1	I	95	LYS
1	I	102	VAL
1	I	116	ASP
1	I	117	LEU
1	I	126	LEU
1	I	129	LEU
1	I	130	THR
1	I	140	LEU
1	I	143	MET
1	I	146	MET
1	I	151	ARG
1	I	163	VAL
1	I	165	PHE
1	I	170	THR
1	I	175	ARG
1	I	182	THR
1	I	186	LEU
1	I	236	THR
1	I	247	LEU
1	I	264	MET
1	I	268	SER
1	I	285	CYS
1	I	289	GLN
1	I	291	ARG
1	I	341	ILE
2	J	35	MET
2	J	37	GLU
2	J	47	LYS
2	J	77	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	HIS
1	A	41	GLN
1	A	50	GLN
1	A	61	ASN
1	A	281	GLN
1	B	18	HIS
1	B	41	GLN

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Mol	Chain	Res	Type
1	B	61	ASN
1	B	98	ASN
1	B	326	ASN
2	C	62	GLN
2	D	62	GLN
1	E	18	HIS
1	E	41	GLN
1	E	61	ASN
1	E	98	ASN
1	E	326	ASN
1	F	18	HIS
1	F	122	GLN
1	F	178	GLN
1	F	222	ASN
1	F	228	GLN
1	F	229	GLN
1	F	267	ASN
1	F	332	GLN
2	G	62	GLN
2	H	62	GLN
1	I	18	HIS
1	I	122	GLN
1	I	178	GLN
1	I	222	ASN
1	I	228	GLN
1	I	267	ASN
1	I	289	GLN
1	I	332	GLN
2	J	62	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 (i)

Of 10 ligands modelled in this entry, 3 are monoatomic - leaving 7 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	PO4	A	364	-	4,4,4	0.50	0	6,6,6	0.28	0
4	PO4	A	365	-	4,4,4	0.54	0	6,6,6	0.30	0
4	PO4	B	363	-	4,4,4	0.39	0	6,6,6	0.30	0
4	PO4	D	7	-	4,4,4	0.54	0	6,6,6	0.28	0
4	PO4	E	364	-	4,4,4	0.54	0	6,6,6	0.29	0
4	PO4	F	363	-	4,4,4	0.42	0	6,6,6	0.29	0
4	PO4	I	364	-	4,4,4	0.55	0	6,6,6	0.28	0

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	PO4	A	364	-	-	0/0/0/0	0/0/0/0
4	PO4	A	365	-	-	0/0/0/0	0/0/0/0
4	PO4	B	363	-	-	0/0/0/0	0/0/0/0
4	PO4	D	7	-	-	0/0/0/0	0/0/0/0
4	PO4	E	364	-	-	0/0/0/0	0/0/0/0
4	PO4	F	363	-	-	0/0/0/0	0/0/0/0
4	PO4	I	364	-	-	0/0/0/0	0/0/0/0

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
4	F	363	PO4	1	0

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	338/362 (93%)	-0.46	1 (0%) 94 84	36, 70, 124, 198	0
1	B	341/362 (94%)	-0.34	2 (0%) 90 73	35, 68, 118, 168	0
1	E	338/362 (93%)	-0.33	1 (0%) 94 84	41, 70, 120, 214	0
1	F	341/362 (94%)	-0.35	0 100 100	41, 75, 117, 154	0
1	I	339/362 (93%)	-0.24	6 (1%) 71 43	43, 76, 126, 249	0
2	C	61/65 (93%)	-0.53	0 100 100	42, 69, 106, 134	0
2	D	61/65 (93%)	-0.40	0 100 100	47, 70, 105, 135	0
2	G	61/65 (93%)	-0.48	0 100 100	46, 71, 108, 137	0
2	H	61/65 (93%)	-0.48	0 100 100	49, 73, 107, 133	0
2	J	61/65 (93%)	-0.35	0 100 100	47, 71, 105, 133	0
All	All	2002/2135 (93%)	-0.36	10 (0%) 91 76	35, 72, 119, 249	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	347	ILE	3.4
1	I	281	GLN	3.3
1	I	348	TYR	3.1
1	I	284	ASN	2.5
1	A	352	ASP	2.5
1	I	351	GLU	2.4
1	E	193	ILE	2.3
1	B	193	ILE	2.2
1	B	352	ASP	2.2
1	I	279	ASN	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
4	PO4	A	365	5/5	0.82	0.31	4.93	111,163,169,181	0
4	PO4	D	7	5/5	0.92	0.37	4.93	121,126,132,137	0
4	PO4	E	364	5/5	0.87	0.25	2.17	112,142,147,153	0
4	PO4	F	363	5/5	0.86	0.23	2.15	117,125,165,167	0
4	PO4	A	364	5/5	0.96	0.23	1.59	111,115,127,129	0
4	PO4	B	363	5/5	0.86	0.24	1.47	94,120,148,162	0
4	PO4	I	364	5/5	0.89	0.16	-0.07	133,136,154,167	0
3	ZN	A	363	1/1	0.99	0.15	-0.63	79,79,79,79	0
3	ZN	E	363	1/1	0.99	0.15	-	82,82,82,82	0
3	ZN	I	363	1/1	0.98	0.04	-	107,107,107,107	1

6.5 Other polymers (i)

There are no such residues in this entry.