Full wwPDB X-ray Structure Validation Report (i)

Sep 5, 2016 – 11:20 AM EDT

PDB ID	:	5HCI
Title	:	GPN-loop GTPase Npa3 in complex with GDP
Authors	:	Niesser, J.; Wagner, F.R.; Kostrewa, D.; Muehlbacher, W.; Cramer, P.
Deposited on	:	2016-01-04
Resolution	:	2.30 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:

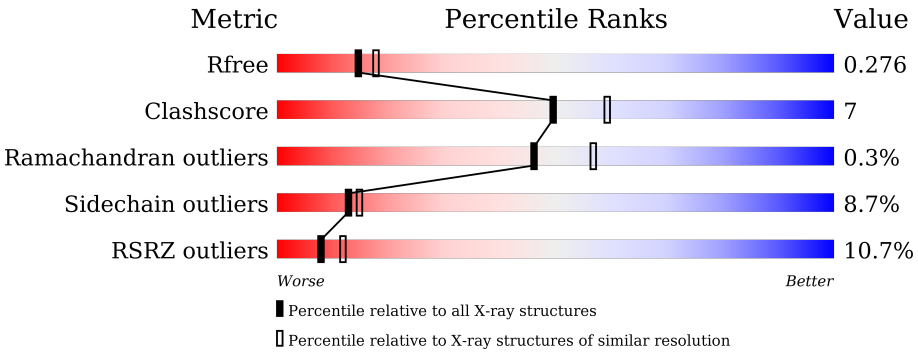
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20027939
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027939

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 2.30 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	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

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	261	4% 81% 15%
1	B	261	14% 75% 17% 5%
1	C	261	12% 72% 19% 6%
1	D	261	8% 84% 12%
1	E	261	7% 81% 15%
1	F	261	17% 82% 12% 5%

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	GOL	C	303	-	-	-	X
4	GOL	E	303	-	-	-	X
4	GOL	E	304	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 12383 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 GPN-loop GTPase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	257	Total	C	N	O	S	0	0	0
			2032	1300	324	391	17			
1	B	258	Total	C	N	O	S	0	0	0
			2042	1306	327	392	17			
1	C	246	Total	C	N	O	S	0	0	0
			1937	1238	309	374	16			
1	D	258	Total	C	N	O	S	0	0	0
			2042	1306	327	392	17			
1	E	259	Total	C	N	O	S	0	0	0
			2052	1312	330	393	17			
1	F	249	Total	C	N	O	S	0	0	0
			1959	1252	314	377	16			

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	LEU	deletion	UNP P47122
A	?	-	ASN	deletion	UNP P47122
A	?	-	GLY	deletion	UNP P47122
A	?	-	ASP	deletion	UNP P47122
A	?	-	ASN	deletion	UNP P47122
A	?	-	GLY	deletion	UNP P47122
A	?	-	LEU	deletion	UNP P47122
A	?	-	GLY	deletion	UNP P47122
A	?	-	SER	deletion	UNP P47122
A	265	LYS	-	expression tag	UNP P47122
A	266	HIS	-	expression tag	UNP P47122
A	267	HIS	-	expression tag	UNP P47122
A	268	HIS	-	expression tag	UNP P47122
A	269	HIS	-	expression tag	UNP P47122
A	270	HIS	-	expression tag	UNP P47122
A	271	HIS	-	expression tag	UNP P47122
B	?	-	LEU	deletion	UNP P47122

Continued on next page...

Continued from previous page...

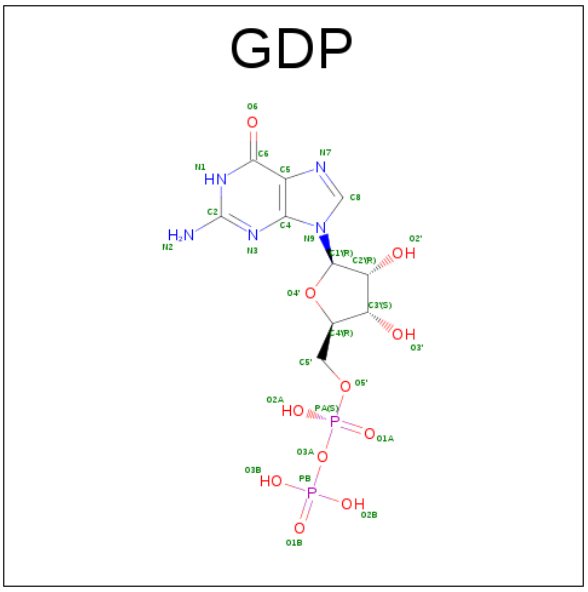
Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	ASN	deletion	UNP P47122
B	?	-	GLY	deletion	UNP P47122
B	?	-	ASP	deletion	UNP P47122
B	?	-	ASN	deletion	UNP P47122
B	?	-	GLY	deletion	UNP P47122
B	?	-	LEU	deletion	UNP P47122
B	?	-	GLY	deletion	UNP P47122
B	?	-	SER	deletion	UNP P47122
B	265	LYS	-	expression tag	UNP P47122
B	266	HIS	-	expression tag	UNP P47122
B	267	HIS	-	expression tag	UNP P47122
B	268	HIS	-	expression tag	UNP P47122
B	269	HIS	-	expression tag	UNP P47122
B	270	HIS	-	expression tag	UNP P47122
B	271	HIS	-	expression tag	UNP P47122
C	?	-	LEU	deletion	UNP P47122
C	?	-	ASN	deletion	UNP P47122
C	?	-	GLY	deletion	UNP P47122
C	?	-	ASP	deletion	UNP P47122
C	?	-	ASN	deletion	UNP P47122
C	?	-	GLY	deletion	UNP P47122
C	?	-	LEU	deletion	UNP P47122
C	?	-	GLY	deletion	UNP P47122
C	?	-	SER	deletion	UNP P47122
C	265	LYS	-	expression tag	UNP P47122
C	266	HIS	-	expression tag	UNP P47122
C	267	HIS	-	expression tag	UNP P47122
C	268	HIS	-	expression tag	UNP P47122
C	269	HIS	-	expression tag	UNP P47122
C	270	HIS	-	expression tag	UNP P47122
C	271	HIS	-	expression tag	UNP P47122
D	?	-	LEU	deletion	UNP P47122
D	?	-	ASN	deletion	UNP P47122
D	?	-	GLY	deletion	UNP P47122
D	?	-	ASP	deletion	UNP P47122
D	?	-	ASN	deletion	UNP P47122
D	?	-	GLY	deletion	UNP P47122
D	?	-	LEU	deletion	UNP P47122
D	?	-	GLY	deletion	UNP P47122
D	?	-	SER	deletion	UNP P47122
D	265	LYS	-	expression tag	UNP P47122
D	266	HIS	-	expression tag	UNP P47122

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	267	HIS	-	expression tag	UNP P47122
D	268	HIS	-	expression tag	UNP P47122
D	269	HIS	-	expression tag	UNP P47122
D	270	HIS	-	expression tag	UNP P47122
D	271	HIS	-	expression tag	UNP P47122
E	?	-	LEU	deletion	UNP P47122
E	?	-	ASN	deletion	UNP P47122
E	?	-	GLY	deletion	UNP P47122
E	?	-	ASP	deletion	UNP P47122
E	?	-	ASN	deletion	UNP P47122
E	?	-	GLY	deletion	UNP P47122
E	?	-	LEU	deletion	UNP P47122
E	?	-	GLY	deletion	UNP P47122
E	?	-	SER	deletion	UNP P47122
E	265	LYS	-	expression tag	UNP P47122
E	266	HIS	-	expression tag	UNP P47122
E	267	HIS	-	expression tag	UNP P47122
E	268	HIS	-	expression tag	UNP P47122
E	269	HIS	-	expression tag	UNP P47122
E	270	HIS	-	expression tag	UNP P47122
E	271	HIS	-	expression tag	UNP P47122
F	?	-	LEU	deletion	UNP P47122
F	?	-	ASN	deletion	UNP P47122
F	?	-	GLY	deletion	UNP P47122
F	?	-	ASP	deletion	UNP P47122
F	?	-	ASN	deletion	UNP P47122
F	?	-	GLY	deletion	UNP P47122
F	?	-	LEU	deletion	UNP P47122
F	?	-	GLY	deletion	UNP P47122
F	?	-	SER	deletion	UNP P47122
F	265	LYS	-	expression tag	UNP P47122
F	266	HIS	-	expression tag	UNP P47122
F	267	HIS	-	expression tag	UNP P47122
F	268	HIS	-	expression tag	UNP P47122
F	269	HIS	-	expression tag	UNP P47122
F	270	HIS	-	expression tag	UNP P47122
F	271	HIS	-	expression tag	UNP P47122

- Molecule 2 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).

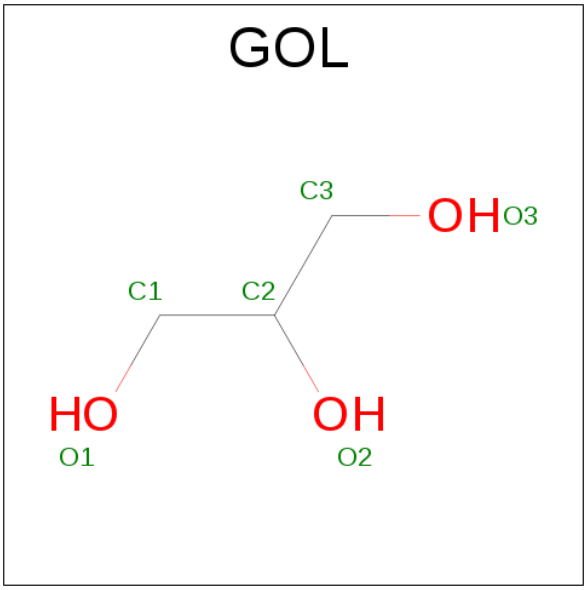


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C N O P 28 10 5 11 2	0	0
2	B	1	Total C N O P 28 10 5 11 2	0	0
2	C	1	Total C N O P 28 10 5 11 2	0	0
2	D	1	Total C N O P 28 10 5 11 2	0	0
2	E	1	Total C N O P 28 10 5 11 2	0	0
2	F	1	Total C N O P 28 10 5 11 2	0	0

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

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

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 6 3 3	0	0
4	C	1	Total C O 6 3 3	0	0
4	E	1	Total C O 6 3 3	0	0
4	E	1	Total C O 6 3 3	0	0

- Molecule 5 is water.

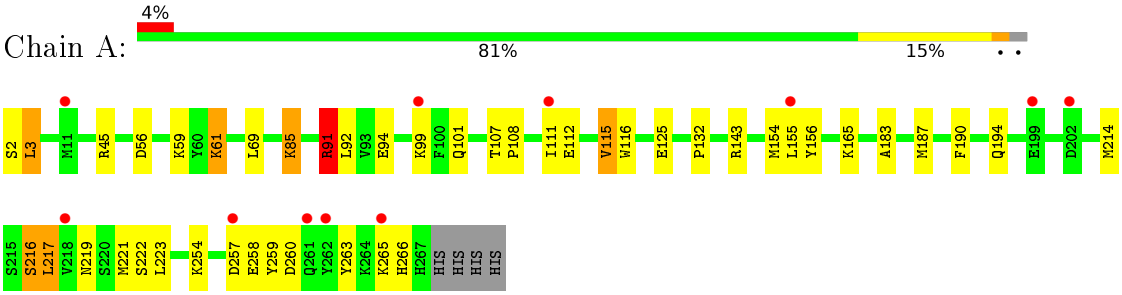
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	33	Total O 33 33	0	0
5	B	30	Total O 30 30	0	0
5	C	16	Total O 16 16	0	0
5	D	16	Total O 16 16	0	0
5	E	21	Total O 21 21	0	0
5	F	5	Total O 5 5	0	0

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.

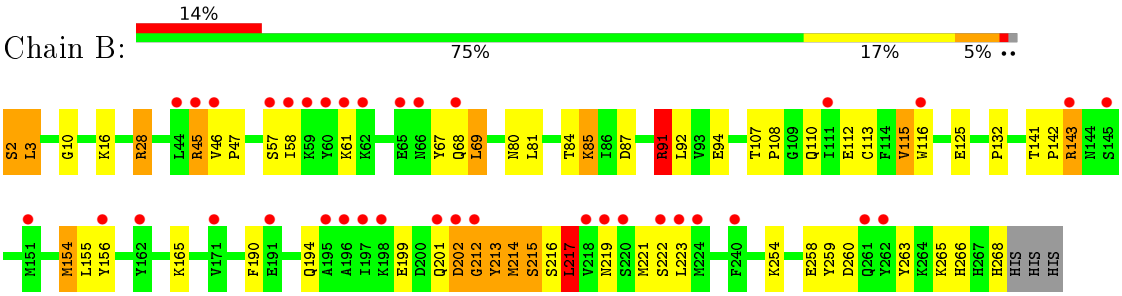
- Molecule 1: GPN-loop GTPase 1

Chain A:



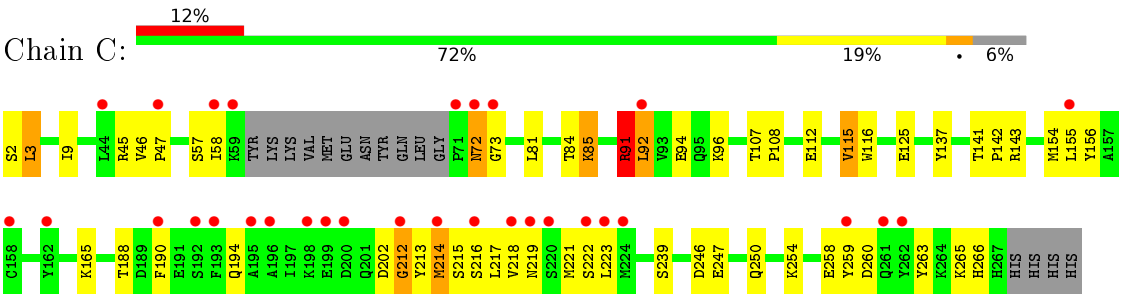
- Molecule 1: GPN-loop GTPase 1

Chain B:



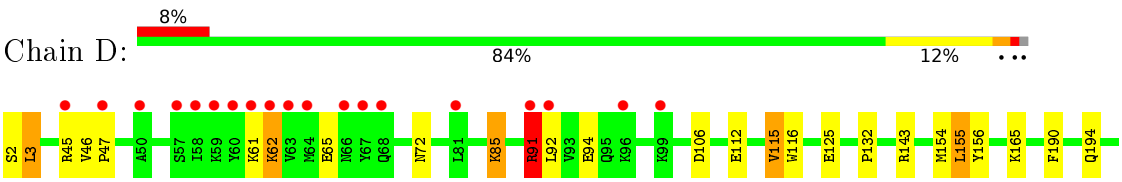
- Molecule 1: GPN-loop GTPase 1

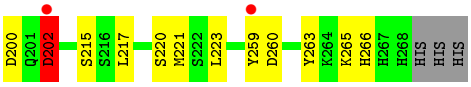
Chain C:



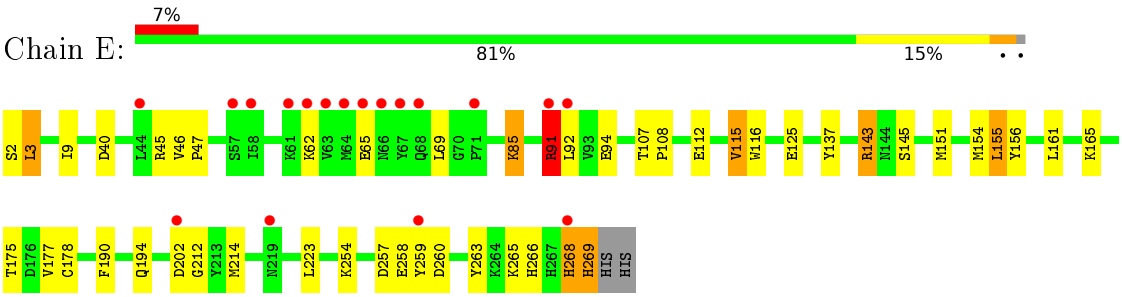
- Molecule 1: GPN-loop GTPase 1

Chain D:

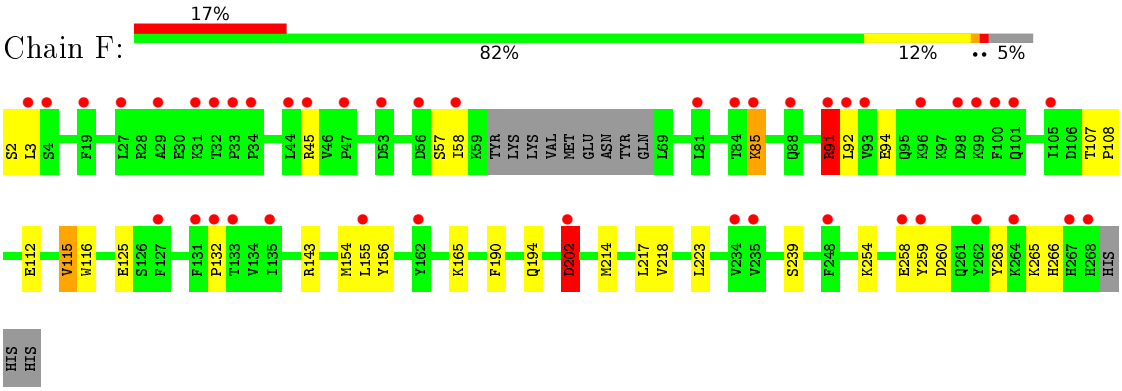




• Molecule 1: GPN-loop GTPase 1



• Molecule 1: GPN-loop GTPase 1



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	107.99Å 119.18Å 347.67Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.25 – 2.30 49.15 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.7 (45.25-2.30) 99.8 (49.15-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [1]	1.50 (at 2.29Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.238 , 0.276 0.239 , 0.276	Depositor DCC
R_{free} test set	1986 reflections (2.00%)	DCC
Wilson B-factor (Å^2)	54.6	Xtriage
Anisotropy	0.533	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 54.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.42$, $< L^2 > = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	12383	wwPDB-VP
Average B, all atoms (Å^2)	82.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.59% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GDP, GOL, MG

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	0.55	0/2075	0.65	2/2806 (0.1%)
1	B	0.58	0/2086	0.90	7/2821 (0.2%)
1	C	0.62	1/1977 (0.1%)	0.70	2/2673 (0.1%)
1	D	0.40	0/2086	0.60	3/2821 (0.1%)
1	E	0.57	0/2097	0.68	3/2836 (0.1%)
1	F	0.38	0/2000	0.58	1/2705 (0.0%)
All	All	0.52	1/12321 (0.0%)	0.69	18/16662 (0.1%)

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	C	0	1
1	D	0	1
1	F	0	1
All	All	0	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	73	GLY	N-CA	-5.39	1.38	1.46

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	45	ARG	NE-CZ-NH1	-20.10	110.25	120.30
1	B	45	ARG	NE-CZ-NH2	19.68	130.14	120.30
1	E	91	ARG	NE-CZ-NH1	10.69	125.64	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	45	ARG	CD-NE-CZ	9.86	137.40	123.60
1	D	91	ARG	NE-CZ-NH1	9.20	124.90	120.30
1	B	91	ARG	NE-CZ-NH1	8.53	124.56	120.30
1	C	91	ARG	NE-CZ-NH1	8.53	124.56	120.30
1	E	91	ARG	NE-CZ-NH2	-8.46	116.07	120.30
1	A	91	ARG	NE-CZ-NH1	7.64	124.12	120.30
1	F	91	ARG	NE-CZ-NH1	7.64	124.12	120.30
1	B	28	ARG	NE-CZ-NH2	-7.36	116.62	120.30
1	B	217	LEU	CA-CB-CG	6.89	131.15	115.30
1	C	3	LEU	CA-CB-CG	5.42	127.77	115.30
1	D	91	ARG	NE-CZ-NH2	-5.33	117.63	120.30
1	E	3	LEU	CA-CB-CG	5.30	127.49	115.30
1	D	3	LEU	CA-CB-CG	5.24	127.35	115.30
1	A	3	LEU	CA-CB-CG	5.20	127.25	115.30
1	B	3	LEU	CA-CB-CG	5.00	126.81	115.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	72	ASN	Peptide
1	D	202	ASP	Peptide
1	F	202	ASP	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	2032	0	2009	22	1
1	B	2042	0	2016	58	0
1	C	1937	0	1914	52	0
1	D	2042	0	2016	20	0
1	E	2052	0	2023	26	1
1	F	1959	0	1933	22	0
2	A	28	0	12	0	0
2	B	28	0	12	0	0
2	C	28	0	12	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	28	0	12	0	0
2	E	28	0	12	0	0
2	F	28	0	12	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
3	E	1	0	0	0	0
3	F	1	0	0	0	0
4	A	6	0	8	1	0
4	C	6	0	8	0	0
4	E	12	0	16	1	0
5	A	33	0	0	2	0
5	B	30	0	0	2	0
5	C	16	0	0	0	0
5	D	16	0	0	1	0
5	E	21	0	0	3	0
5	F	5	0	0	0	0
All	All	12383	0	12015	173	1

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 7.

All (173) 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:91:ARG:HG3	1:D:202:ASP:HB3	1.23	1.13
1:C:202:ASP:O	1:C:213:TYR:N	1.85	1.07
1:C:91:ARG:HG3	1:F:202:ASP:HB3	1.48	0.94
1:B:143:ARG:NH2	5:B:401:HOH:O	2.01	0.92
1:C:91:ARG:CG	1:F:202:ASP:HB3	2.08	0.82
1:C:214:MET:HB3	1:C:217:LEU:HD13	1.62	0.80
1:C:91:ARG:HG3	1:F:202:ASP:CB	2.12	0.79
1:B:28:ARG:HE	1:C:250:GLN:CD	1.91	0.74
1:B:28:ARG:HH22	1:C:247:GLU:N	1.86	0.73
1:B:45:ARG:NH2	1:C:188:THR:OG1	2.24	0.71
1:F:190:PHE:HD2	1:F:194:GLN:HE21	1.38	0.71
1:B:28:ARG:HE	1:C:250:GLN:NE2	1.87	0.71
1:B:190:PHE:HD2	1:B:194:GLN:HE21	1.39	0.70
1:C:190:PHE:HD2	1:C:194:GLN:HE21	1.40	0.70
1:B:199:GLU:OE2	5:B:402:HOH:O	2.10	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:56:ASP:OD2	5:A:401:HOH:O	2.10	0.69
1:E:263:TYR:OH	5:E:401:HOH:O	2.10	0.69
1:B:212:GLY:O	1:B:215:SER:N	2.27	0.67
1:D:91:ARG:HH11	1:D:91:ARG:HG3	1.60	0.67
1:E:190:PHE:HD2	1:E:194:GLN:HE21	1.43	0.66
1:B:28:ARG:HH22	1:C:246:ASP:C	2.00	0.66
1:F:91:ARG:HH11	1:F:91:ARG:HG3	1.61	0.65
1:B:45:ARG:HB3	1:C:188:THR:CG2	2.26	0.65
1:A:91:ARG:HH11	1:A:91:ARG:HG3	1.62	0.65
1:B:91:ARG:HG3	1:D:202:ASP:CB	2.15	0.65
1:D:190:PHE:HD2	1:D:194:GLN:HE21	1.45	0.64
1:C:217:LEU:HB3	1:C:221:MET:SD	2.38	0.64
1:C:214:MET:N	1:C:214:MET:SD	2.71	0.63
1:A:190:PHE:HD2	1:A:194:GLN:HE21	1.46	0.62
1:A:59:LYS:HD2	1:A:61:LYS:HZ2	1.64	0.62
1:B:217:LEU:O	1:B:221:MET:HG3	1.99	0.62
1:A:99:LYS:HG3	1:B:2:SER:OG	1.99	0.62
1:E:91:ARG:HG3	1:E:91:ARG:HH11	1.66	0.61
1:B:45:ARG:HD2	1:C:188:THR:HG21	1.82	0.61
1:B:115:VAL:HG22	1:B:116:TRP:CE3	2.36	0.60
1:B:28:ARG:NH2	1:C:246:ASP:C	2.56	0.59
1:B:201:GLN:HG2	1:B:213:TYR:H	1.68	0.59
1:B:212:GLY:HA3	1:B:215:SER:HB3	1.84	0.59
1:C:214:MET:O	1:C:217:LEU:HB2	2.02	0.59
1:A:115:VAL:HG22	1:A:116:TRP:CE3	2.37	0.59
1:E:115:VAL:HG22	1:E:116:TRP:CE3	2.36	0.59
1:E:257:ASP:HB3	4:E:303:GOL:H31	1.84	0.58
1:B:28:ARG:NH2	1:C:247:GLU:N	2.52	0.58
1:F:115:VAL:HG22	1:F:116:TRP:CE3	2.39	0.58
1:B:202:ASP:O	1:B:212:GLY:C	2.42	0.56
1:B:201:GLN:HG2	1:B:213:TYR:HB3	1.86	0.56
1:C:212:GLY:HA2	1:C:215:SER:HB3	1.86	0.56
1:B:45:ARG:HB3	1:C:188:THR:HG21	1.86	0.56
1:D:115:VAL:HG22	1:D:116:TRP:CE3	2.41	0.56
1:C:91:ARG:HH11	1:C:91:ARG:HG3	1.70	0.56
1:A:91:ARG:HH11	1:A:91:ARG:CG	2.19	0.55
1:F:165:LYS:HE3	1:F:266:HIS:HD2	1.72	0.54
1:E:91:ARG:CG	1:E:91:ARG:HH11	2.20	0.54
1:F:91:ARG:HH11	1:F:91:ARG:CG	2.19	0.54
1:D:165:LYS:HE3	1:D:266:HIS:HD2	1.72	0.54
1:D:91:ARG:HH11	1:D:91:ARG:CG	2.20	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:165:LYS:HE3	1:E:266:HIS:HD2	1.73	0.53
1:C:115:VAL:HG22	1:C:116:TRP:CE3	2.42	0.53
1:A:165:LYS:HE3	1:A:266:HIS:HD2	1.73	0.52
1:F:214:MET:O	1:F:218:VAL:HG23	2.10	0.52
1:B:80:ASN:HB3	1:E:177:VAL:O	2.10	0.51
1:E:254:LYS:NZ	1:E:258:GLU:OE2	2.34	0.51
1:B:165:LYS:HE3	1:B:266:HIS:HD2	1.76	0.51
1:B:212:GLY:O	1:B:214:MET:N	2.44	0.51
1:C:165:LYS:HE3	1:C:266:HIS:HD2	1.75	0.51
1:B:91:ARG:CG	1:B:91:ARG:HH11	2.24	0.50
1:A:216:SER:O	1:A:219:ASN:HB2	2.11	0.50
1:B:91:ARG:HG3	1:B:91:ARG:HH11	1.77	0.50
1:D:265:LYS:HG3	1:D:266:HIS:ND1	2.26	0.50
1:C:91:ARG:HG3	1:F:202:ASP:CG	2.30	0.50
1:F:265:LYS:HG3	1:F:266:HIS:ND1	2.27	0.50
1:C:91:ARG:HH11	1:C:91:ARG:CG	2.24	0.50
1:B:28:ARG:NE	1:C:250:GLN:NE2	2.56	0.49
1:C:265:LYS:HG3	1:C:266:HIS:ND1	2.28	0.49
1:D:155:LEU:HD23	1:E:155:LEU:HD23	1.94	0.48
1:B:28:ARG:NH2	1:C:246:ASP:HB3	2.29	0.48
1:D:165:LYS:HE2	1:D:266:HIS:HB3	1.96	0.48
1:C:215:SER:O	1:C:218:VAL:N	2.46	0.48
1:E:161:LEU:HD21	5:E:401:HOH:O	2.13	0.47
1:E:202:ASP:OD1	1:E:202:ASP:N	2.47	0.47
1:A:265:LYS:HG3	1:A:266:HIS:ND1	2.29	0.47
1:B:110:GLN:HB2	1:B:113:CYS:SG	2.54	0.47
1:E:40:ASP:OD2	5:E:402:HOH:O	2.20	0.47
1:E:165:LYS:HE2	1:E:266:HIS:HB3	1.96	0.47
1:F:202:ASP:OD1	1:F:202:ASP:N	2.47	0.47
1:B:201:GLN:HE21	1:B:213:TYR:HB3	1.80	0.47
1:E:175:THR:HA	1:E:178:CYS:O	2.15	0.47
1:F:254:LYS:NZ	1:F:258:GLU:OE2	2.38	0.47
1:E:265:LYS:HG3	1:E:266:HIS:ND1	2.29	0.47
1:B:265:LYS:HG3	1:B:266:HIS:ND1	2.29	0.47
1:F:165:LYS:HE2	1:F:266:HIS:HB3	1.97	0.47
1:B:45:ARG:HB3	1:C:188:THR:HG23	1.95	0.46
1:C:222:SER:OG	1:C:223:LEU:N	2.48	0.46
1:D:220:SER:HB2	1:E:156:TYR:CE2	2.50	0.46
1:A:85:LYS:N	1:A:85:LYS:HD2	2.30	0.46
1:C:91:ARG:HG2	1:F:202:ASP:HB3	1.92	0.46
1:B:222:SER:OG	1:B:223:LEU:N	2.47	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:141:THR:HB	1:C:142:PRO:HD3	1.96	0.46
1:B:254:LYS:NZ	1:B:258:GLU:OE2	2.38	0.46
1:F:223:LEU:HD23	1:F:223:LEU:HA	1.79	0.46
1:D:259:TYR:HA	1:D:263:TYR:HB2	1.97	0.46
1:B:141:THR:HB	1:B:142:PRO:HD3	1.97	0.46
1:E:151:MET:O	1:E:155:LEU:HD22	2.15	0.46
1:C:212:GLY:HA2	1:C:215:SER:CB	2.46	0.46
1:C:259:TYR:HA	1:C:263:TYR:HB2	1.97	0.46
1:A:165:LYS:HE2	1:A:266:HIS:HB3	1.98	0.45
1:B:201:GLN:HE21	1:B:213:TYR:CB	2.29	0.45
1:B:202:ASP:O	1:B:213:TYR:N	2.49	0.45
1:B:259:TYR:HA	1:B:263:TYR:HB2	1.97	0.45
1:C:85:LYS:N	1:C:85:LYS:HD2	2.31	0.45
1:D:62:LYS:HE3	1:D:62:LYS:HB2	1.78	0.45
1:E:259:TYR:HA	1:E:263:TYR:HB2	1.98	0.45
1:E:46:VAL:HA	1:E:47:PRO:HD3	1.80	0.45
1:B:81:LEU:O	1:B:84:THR:HB	2.15	0.45
1:B:165:LYS:HE2	1:B:266:HIS:HB3	1.98	0.45
1:C:165:LYS:HE2	1:C:266:HIS:HB3	1.98	0.45
1:F:259:TYR:HA	1:F:263:TYR:HB2	1.98	0.44
1:A:259:TYR:HA	1:A:263:TYR:HB2	1.99	0.44
1:C:219:ASN:O	1:C:222:SER:HB3	2.17	0.44
1:B:87:ASP:CG	1:E:143:ARG:HH22	2.21	0.44
1:D:106:ASP:OD1	5:D:402:HOH:O	2.21	0.44
1:F:85:LYS:N	1:F:85:LYS:HD2	2.33	0.44
1:C:84:THR:HG22	1:C:85:LYS:HD2	2.00	0.44
1:E:85:LYS:HD2	1:E:85:LYS:N	2.33	0.44
1:C:46:VAL:HA	1:C:47:PRO:HD3	1.84	0.44
1:D:85:LYS:N	1:D:85:LYS:HD2	2.33	0.44
1:B:84:THR:HG22	1:B:85:LYS:HD2	1.99	0.43
1:E:268:HIS:CD2	1:E:269:HIS:HB3	2.53	0.43
1:A:254:LYS:NZ	1:A:258:GLU:OE2	2.38	0.43
1:C:107:THR:HB	1:C:108:PRO:HD2	2.00	0.43
1:F:57:SER:OG	1:F:58:ILE:HD12	2.18	0.43
1:C:9:ILE:O	1:C:137:TYR:HA	2.18	0.43
1:F:239:SER:N	2:F:301:GDP:O6	2.51	0.43
1:B:107:THR:HB	1:B:108:PRO:HD2	1.99	0.43
1:B:28:ARG:NH2	1:C:247:GLU:HA	2.33	0.43
1:D:46:VAL:HA	1:D:47:PRO:HD3	1.82	0.43
1:C:81:LEU:O	1:C:84:THR:HB	2.19	0.43
1:C:217:LEU:O	1:C:221:MET:HG3	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:91:ARG:NH2	1:D:200:ASP:O	2.52	0.42
1:A:219:ASN:O	1:A:222:SER:HB3	2.19	0.42
1:B:57:SER:OG	1:B:58:ILE:HD12	2.19	0.42
1:C:202:ASP:OD1	1:C:202:ASP:N	2.50	0.42
1:B:154:MET:CE	1:B:154:MET:HA	2.49	0.42
1:A:107:THR:HB	1:A:108:PRO:HD2	2.02	0.42
1:A:183:ALA:O	1:A:187:MET:HG3	2.19	0.42
1:B:132:PRO:HA	1:B:259:TYR:CE1	2.55	0.42
1:B:219:ASN:O	1:B:222:SER:HB3	2.19	0.42
1:B:69:LEU:HD13	1:B:69:LEU:HA	1.86	0.42
1:C:254:LYS:NZ	1:C:258:GLU:OE2	2.39	0.42
1:C:239:SER:N	2:C:301:GDP:O6	2.52	0.42
1:E:223:LEU:HD23	1:E:223:LEU:HA	1.88	0.42
1:A:111:ILE:HA	5:A:417:HOH:O	2.20	0.41
1:C:223:LEU:HD23	1:C:223:LEU:HA	1.90	0.41
1:B:85:LYS:HD2	1:B:85:LYS:N	2.35	0.41
1:C:190:PHE:CZ	1:C:222:SER:HA	2.55	0.41
1:F:132:PRO:HA	1:F:259:TYR:CE1	2.55	0.41
1:E:107:THR:HB	1:E:108:PRO:HD2	2.01	0.41
1:C:57:SER:OG	1:C:58:ILE:HD12	2.21	0.41
1:C:92:LEU:O	1:C:96:LYS:HG2	2.20	0.41
1:A:223:LEU:HA	1:A:223:LEU:HD23	1.79	0.41
1:B:10:GLY:N	1:B:16:LYS:HD3	2.35	0.41
1:B:67:TYR:HB3	1:B:69:LEU:HD22	2.02	0.41
1:B:46:VAL:HA	1:B:47:PRO:HD3	1.81	0.41
1:D:223:LEU:HA	1:D:223:LEU:HD23	1.81	0.41
1:E:9:ILE:O	1:E:137:TYR:HA	2.21	0.41
1:A:132:PRO:HA	1:A:259:TYR:CE1	2.56	0.41
1:F:107:THR:HB	1:F:108:PRO:HD2	2.03	0.41
1:A:101:GLN:CD	4:A:303:GOL:H32	2.41	0.40
1:A:217:LEU:HD12	1:A:221:MET:SD	2.61	0.40
1:B:190:PHE:CZ	1:B:222:SER:HA	2.57	0.40
1:D:217:LEU:O	1:D:221:MET:HG3	2.21	0.40
1:B:202:ASP:OD1	1:B:202:ASP:N	2.48	0.40
1:D:132:PRO:HA	1:D:259:TYR:CE1	2.56	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:257:ASP:O	1:E:91:ARG:NH2[5_455]	2.13	0.07

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	255/261 (98%)	251 (98%)	4 (2%)	0	100	100
1	B	256/261 (98%)	250 (98%)	4 (2%)	2 (1%)	24	27
1	C	242/261 (93%)	236 (98%)	5 (2%)	1 (0%)	39	48
1	D	256/261 (98%)	252 (98%)	4 (2%)	0	100	100
1	E	257/261 (98%)	252 (98%)	4 (2%)	1 (0%)	39	48
1	F	245/261 (94%)	241 (98%)	4 (2%)	0	100	100
All	All	1511/1566 (96%)	1482 (98%)	25 (2%)	4 (0%)	46	57

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	212	GLY
1	C	212	GLY
1	B	213	TYR
1	E	212	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	231/235 (98%)	211 (91%)	20 (9%)	13	15
1	B	232/235 (99%)	209 (90%)	23 (10%)	10	11
1	C	221/235 (94%)	203 (92%)	18 (8%)	15	18

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	D	232/235 (99%)	211 (91%)	21 (9%)	12 13
1	E	233/235 (99%)	212 (91%)	21 (9%)	12 14
1	F	223/235 (95%)	206 (92%)	17 (8%)	16 20
All	All	1372/1410 (97%)	1252 (91%)	120 (9%)	13 15

All (120) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	SER
1	A	3	LEU
1	A	45	ARG
1	A	61	LYS
1	A	69	LEU
1	A	85	LYS
1	A	91	ARG
1	A	92	LEU
1	A	94	GLU
1	A	112	GLU
1	A	115	VAL
1	A	125	GLU
1	A	143	ARG
1	A	154	MET
1	A	155	LEU
1	A	156	TYR
1	A	214	MET
1	A	216	SER
1	A	217	LEU
1	A	260	ASP
1	B	2	SER
1	B	3	LEU
1	B	61	LYS
1	B	68	GLN
1	B	69	LEU
1	B	85	LYS
1	B	91	ARG
1	B	92	LEU
1	B	94	GLU
1	B	112	GLU
1	B	115	VAL
1	B	125	GLU
1	B	143	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	154	MET
1	B	155	LEU
1	B	156	TYR
1	B	202	ASP
1	B	214	MET
1	B	215	SER
1	B	216	SER
1	B	217	LEU
1	B	260	ASP
1	B	268	HIS
1	C	2	SER
1	C	3	LEU
1	C	45	ARG
1	C	72	ASN
1	C	85	LYS
1	C	91	ARG
1	C	92	LEU
1	C	94	GLU
1	C	112	GLU
1	C	115	VAL
1	C	125	GLU
1	C	143	ARG
1	C	154	MET
1	C	155	LEU
1	C	156	TYR
1	C	214	MET
1	C	216	SER
1	C	260	ASP
1	D	2	SER
1	D	3	LEU
1	D	45	ARG
1	D	61	LYS
1	D	62	LYS
1	D	65	GLU
1	D	72	ASN
1	D	85	LYS
1	D	91	ARG
1	D	92	LEU
1	D	94	GLU
1	D	112	GLU
1	D	115	VAL
1	D	125	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	143	ARG
1	D	154	MET
1	D	155	LEU
1	D	156	TYR
1	D	202	ASP
1	D	215	SER
1	D	260	ASP
1	E	2	SER
1	E	3	LEU
1	E	45	ARG
1	E	62	LYS
1	E	65	GLU
1	E	69	LEU
1	E	85	LYS
1	E	91	ARG
1	E	92	LEU
1	E	94	GLU
1	E	112	GLU
1	E	115	VAL
1	E	125	GLU
1	E	143	ARG
1	E	145	SER
1	E	154	MET
1	E	155	LEU
1	E	214	MET
1	E	260	ASP
1	E	268	HIS
1	E	269	HIS
1	F	2	SER
1	F	3	LEU
1	F	45	ARG
1	F	85	LYS
1	F	91	ARG
1	F	92	LEU
1	F	94	GLU
1	F	112	GLU
1	F	115	VAL
1	F	125	GLU
1	F	143	ARG
1	F	154	MET
1	F	155	LEU
1	F	156	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	202	ASP
1	F	217	LEU
1	F	260	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	194	GLN
1	B	194	GLN
1	B	201	GLN
1	C	194	GLN
1	C	250	GLN
1	D	194	GLN
1	E	194	GLN
1	F	194	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 16 ligands modelled in this entry, 6 are monoatomic - leaving 10 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	$\#\|Z\|>2$
2	GDP	A	301	3	24,30,30	1.14	2 (8%)	26,47,47	2.22	8 (30%)
4	GOL	A	303	-	5,5,5	0.32	0	5,5,5	0.60	0
2	GDP	B	301	3	24,30,30	1.20	2 (8%)	26,47,47	2.13	7 (26%)
2	GDP	C	301	-	24,30,30	1.31	2 (8%)	26,47,47	1.87	4 (15%)
4	GOL	C	303	-	5,5,5	0.35	0	5,5,5	0.29	0
2	GDP	D	301	3	24,30,30	1.25	2 (8%)	26,47,47	1.91	5 (19%)
2	GDP	E	301	3	24,30,30	1.28	2 (8%)	26,47,47	2.19	8 (30%)
4	GOL	E	303	-	5,5,5	0.32	0	5,5,5	0.22	0
4	GOL	E	304	-	5,5,5	0.34	0	5,5,5	0.57	0
2	GDP	F	301	3	24,30,30	1.16	2 (8%)	26,47,47	2.00	5 (19%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GDP	A	301	3	-	0/12/32/32	0/3/3/3
4	GOL	A	303	-	-	0/4/4/4	0/0/0/0
2	GDP	B	301	3	-	0/12/32/32	0/3/3/3
2	GDP	C	301	-	-	0/12/32/32	0/3/3/3
4	GOL	C	303	-	-	0/4/4/4	0/0/0/0
2	GDP	D	301	3	-	0/12/32/32	0/3/3/3
2	GDP	E	301	3	-	0/12/32/32	0/3/3/3
4	GOL	E	303	-	-	0/4/4/4	0/0/0/0
4	GOL	E	304	-	-	0/4/4/4	0/0/0/0
2	GDP	F	301	3	-	0/12/32/32	0/3/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	301	GDP	C5-C4	2.69	1.46	1.40
2	C	301	GDP	C5-C4	2.88	1.47	1.40
2	A	301	GDP	C5-C4	2.93	1.47	1.40
2	B	301	GDP	C5-C4	3.10	1.47	1.40
2	F	301	GDP	C5-C4	3.17	1.47	1.40
2	D	301	GDP	C5-C4	3.35	1.48	1.40
2	F	301	GDP	C6-C5	3.42	1.48	1.41
2	A	301	GDP	C6-C5	3.57	1.48	1.41
2	B	301	GDP	C6-C5	3.63	1.48	1.41
2	D	301	GDP	C6-C5	3.79	1.49	1.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	301	GDP	C6-C5	3.85	1.49	1.41
2	C	301	GDP	C6-C5	4.52	1.50	1.41

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	301	GDP	C5-C6-N1	-5.43	116.42	123.52
2	B	301	GDP	C5-C6-N1	-5.27	116.63	123.52
2	F	301	GDP	C5-C6-N1	-4.50	117.65	123.52
2	E	301	GDP	N3-C2-N1	-4.43	121.53	127.56
2	C	301	GDP	N3-C2-N1	-4.18	121.88	127.56
2	E	301	GDP	C5'-C4'-C3'	-4.16	99.11	115.20
2	D	301	GDP	C5-C6-N1	-4.10	118.16	123.52
2	C	301	GDP	C5-C6-N1	-4.04	118.25	123.52
2	E	301	GDP	C6-C5-C4	-3.98	116.31	120.86
2	F	301	GDP	N3-C2-N1	-3.80	122.38	127.56
2	F	301	GDP	C6-C5-C4	-3.79	116.53	120.86
2	A	301	GDP	N3-C2-N1	-3.68	122.55	127.56
2	B	301	GDP	C1'-N9-C4	-3.40	123.02	126.81
2	E	301	GDP	C5-C6-N1	-3.38	119.11	123.52
2	A	301	GDP	C2'-C1'-N9	-3.29	104.65	113.47
2	D	301	GDP	C6-C5-C4	-3.25	117.14	120.86
2	C	301	GDP	C6-C5-C4	-3.06	117.36	120.86
2	D	301	GDP	N3-C2-N1	-3.05	123.40	127.56
2	B	301	GDP	N3-C2-N1	-2.86	123.66	127.56
2	E	301	GDP	C4'-O4'-C1'	-2.85	106.63	109.64
2	B	301	GDP	C6-C5-C4	-2.77	117.69	120.86
2	F	301	GDP	C1'-N9-C4	-2.57	123.94	126.81
2	A	301	GDP	C6-C5-C4	-2.45	118.06	120.86
2	A	301	GDP	O2B-PB-O1B	-2.13	103.68	110.63
2	B	301	GDP	O3B-PB-O2B	2.05	114.96	107.44
2	B	301	GDP	C2'-C3'-C4'	2.06	106.84	102.64
2	E	301	GDP	O4'-C4'-C3'	2.13	109.48	105.16
2	A	301	GDP	O2A-PA-O3A	2.15	114.49	105.27
2	E	301	GDP	N2-C2-N1	2.26	120.94	117.20
2	A	301	GDP	O4'-C1'-N9	2.79	113.38	108.11
2	D	301	GDP	O4'-C1'-N9	3.91	115.48	108.11
2	E	301	GDP	C6-N1-C2	5.00	121.74	115.88
2	D	301	GDP	C6-N1-C2	5.23	122.01	115.88
2	C	301	GDP	C6-N1-C2	5.52	122.36	115.88
2	B	301	GDP	C6-N1-C2	5.81	122.69	115.88
2	F	301	GDP	C6-N1-C2	6.19	123.13	115.88

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	301	GDP	C6-N1-C2	6.34	123.31	115.88

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	303	GOL	1	0
2	C	301	GDP	1	0
4	E	303	GOL	1	0
2	F	301	GDP	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	257/261 (98%)	0.39	11 (4%) 39 48	42, 60, 106, 198	0
1	B	258/261 (98%)	1.01	37 (14%) 4 6	44, 69, 146, 237	0
1	C	246/261 (94%)	0.86	31 (12%) 5 8	48, 72, 158, 280	0
1	D	258/261 (98%)	0.63	21 (8%) 15 21	56, 83, 135, 186	0
1	E	259/261 (99%)	0.50	18 (6%) 20 27	44, 63, 127, 211	0
1	F	249/261 (95%)	1.19	45 (18%) 2 3	55, 104, 146, 195	0
All	All	1527/1566 (97%)	0.76	163 (10%) 8 12	42, 74, 141, 280	0

All (163) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	220	SER	14.8
1	D	67	TYR	11.2
1	B	223	LEU	10.0
1	C	223	LEU	9.8
1	D	63	VAL	9.0
1	C	222	SER	8.9
1	C	198	LYS	8.7
1	B	219	ASN	8.5
1	C	58	ILE	8.2
1	B	198	LYS	7.9
1	C	219	ASN	7.5
1	D	60	TYR	7.4
1	F	93	VAL	6.8
1	D	64	MET	6.5
1	D	66	ASN	6.4
1	F	202	ASP	6.3
1	F	3	LEU	6.2
1	E	66	ASN	6.0
1	D	58	ILE	5.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	220	SER	5.7
1	F	32	THR	5.4
1	F	58	ILE	5.0
1	C	190	PHE	4.8
1	E	63	VAL	4.8
1	E	61	LYS	4.8
1	F	259	TYR	4.7
1	E	68	GLN	4.7
1	C	72	ASN	4.7
1	F	131	PHE	4.7
1	B	195	ALA	4.6
1	B	58	ILE	4.5
1	F	91	ARG	4.5
1	D	99	LYS	4.4
1	E	92	LEU	4.4
1	B	59	LYS	4.4
1	E	62	LYS	4.3
1	F	84	THR	4.2
1	F	268	HIS	4.2
1	C	195	ALA	4.2
1	A	202	ASP	4.2
1	C	224	MET	4.2
1	C	59	LYS	4.2
1	F	33	PRO	4.2
1	F	262	TYR	4.1
1	F	105	ILE	4.1
1	B	262	TYR	4.0
1	F	4	SER	4.0
1	F	27	LEU	4.0
1	B	212	GLY	4.0
1	E	268	HIS	4.0
1	D	59	LYS	4.0
1	F	85	LYS	4.0
1	B	45	ARG	3.9
1	F	234	VAL	3.9
1	C	212	GLY	3.8
1	F	98	ASP	3.8
1	C	73	GLY	3.8
1	C	218	VAL	3.8
1	C	192	SER	3.8
1	B	162	TYR	3.7
1	B	218	VAL	3.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	222	SER	3.6
1	B	224	MET	3.6
1	F	81	LEU	3.6
1	C	214	MET	3.5
1	C	44	LEU	3.5
1	F	248	PHE	3.4
1	F	92	LEU	3.4
1	F	47	PRO	3.4
1	F	44	LEU	3.4
1	C	199	GLU	3.3
1	E	65	GLU	3.3
1	B	196	ALA	3.2
1	B	46	VAL	3.2
1	D	45	ARG	3.2
1	D	62	LYS	3.2
1	C	196	ALA	3.2
1	A	257	ASP	3.2
1	E	57	SER	3.1
1	D	92	LEU	3.1
1	F	127	PHE	3.1
1	A	199	GLU	3.0
1	B	202	ASP	3.0
1	F	132	PRO	2.9
1	E	58	ILE	2.9
1	A	262	TYR	2.9
1	D	96	LYS	2.8
1	F	258	GLU	2.8
1	B	68	GLN	2.8
1	F	100	PHE	2.8
1	D	50	ALA	2.8
1	D	61	LYS	2.8
1	D	202	ASP	2.7
1	C	216	SER	2.7
1	D	91	ARG	2.7
1	E	202	ASP	2.7
1	B	197	ILE	2.7
1	B	60	TYR	2.7
1	F	99	LYS	2.7
1	B	66	ASN	2.6
1	A	111	ILE	2.6
1	F	19	PHE	2.6
1	D	259	TYR	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	201	GLN	2.6
1	F	29	ALA	2.6
1	B	151	MET	2.5
1	D	68	GLN	2.5
1	B	240	PHE	2.5
1	C	71	PRO	2.5
1	F	88	GLN	2.5
1	E	219	ASN	2.5
1	B	145	SER	2.5
1	C	47	PRO	2.5
1	F	133	THR	2.5
1	D	57	SER	2.5
1	E	67	TYR	2.5
1	A	265	LYS	2.5
1	F	162	TYR	2.4
1	B	116	TRP	2.4
1	A	155	LEU	2.4
1	C	155	LEU	2.4
1	E	44	LEU	2.4
1	D	47	PRO	2.4
1	B	156	TYR	2.4
1	F	267	HIS	2.4
1	A	99	LYS	2.3
1	F	101	GLN	2.3
1	B	191	GLU	2.3
1	F	96	LYS	2.3
1	B	143	ARG	2.3
1	B	44	LEU	2.3
1	F	235	VAL	2.3
1	F	264	LYS	2.3
1	E	64	MET	2.2
1	A	11	MET	2.2
1	A	218	VAL	2.2
1	B	61	LYS	2.2
1	F	34	PRO	2.2
1	B	111	ILE	2.2
1	F	135	ILE	2.2
1	C	193	PHE	2.2
1	B	261	GLN	2.2
1	F	45	ARG	2.2
1	F	31	LYS	2.2
1	F	155	LEU	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	53	ASP	2.2
1	B	62	LYS	2.1
1	C	162	TYR	2.1
1	D	81	LEU	2.1
1	C	158	CYS	2.1
1	B	57	SER	2.1
1	B	65	GLU	2.1
1	A	261	GLN	2.1
1	C	261	GLN	2.1
1	F	56	ASP	2.1
1	C	259	TYR	2.1
1	E	259	TYR	2.1
1	E	71	PRO	2.0
1	C	200	ASP	2.0
1	B	171	VAL	2.0
1	C	262	TYR	2.0
1	C	92	LEU	2.0
1	E	91	ARG	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	GOL	E	303	6/6	0.59	0.46	4.87	91,102,106,108	0
4	GOL	C	303	6/6	0.73	0.22	3.88	90,102,119,125	0
4	GOL	E	304	6/6	0.86	0.26	3.42	69,98,110,124	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	GDP	E	301	28/28	0.95	0.20	0.62	54,61,86,110	0
2	GDP	A	301	28/28	0.98	0.18	0.26	57,59,77,79	0
2	GDP	C	301	28/28	0.93	0.16	-0.01	45,66,77,84	0
2	GDP	B	301	28/28	0.97	0.14	-0.87	51,53,63,65	0
3	MG	B	302	1/1	0.94	0.12	-1.14	52,52,52,52	0
2	GDP	D	301	28/28	0.96	0.11	-1.38	55,68,91,136	0
2	GDP	F	301	28/28	0.93	0.13	-1.70	71,93,103,114	0
3	MG	C	302	1/1	0.96	0.19	-	63,63,63,63	0
3	MG	A	302	1/1	0.94	0.24	-	55,55,55,55	0
3	MG	D	302	1/1	0.93	0.06	-	65,65,65,65	0
4	GOL	A	303	6/6	0.64	0.48	-	104,119,129,129	0
3	MG	E	302	1/1	0.97	0.07	-	61,61,61,61	0
3	MG	F	302	1/1	0.97	0.21	-	85,85,85,85	0

6.5 Other polymers

There are no such residues in this entry.