Full wwPDB X-ray Structure Validation Report (i)

Feb 19, 2016 – 10:04 PM GMT

PDB ID	:	5CA9
Title	:	Structures of the candida albicans sey1p GTPase in complex with GDPAlF4-
Authors	:	Yan, L.
Deposited on	:	2015-06-29
Resolution	:	2.80 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 (i) symbol.

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

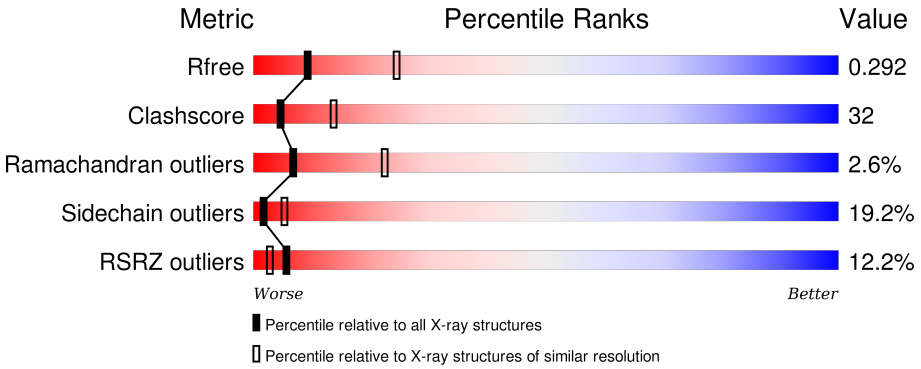
MolProbity	:	4.02b-467
Mogul	:	unknown
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026982
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20026982

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 2.80 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	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

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 <=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	692	12% 45% 38% 10% • 5%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 5452 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 Protein SEY1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	656	Total	C	N	O	S	0	0	0
			5303	3390	877	1025	11			

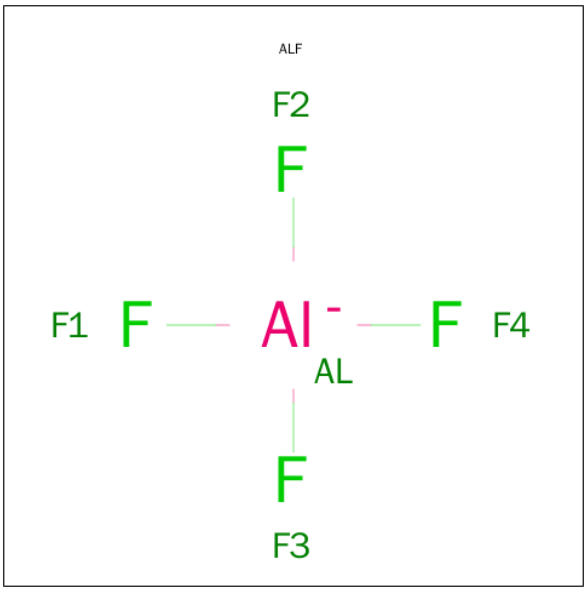
There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	89	LEU	SER	see sequence details	UNP Q9C0L9
A	221	LEU	SER	see sequence details	UNP Q9C0L9
A	270	GLY	ASP	see sequence details	UNP Q9C0L9
A	337	THR	ALA	see sequence details	UNP Q9C0L9
A	479	VAL	ILE	see sequence details	UNP Q9C0L9
A	665	LEU	SER	see sequence details	UNP Q9C0L9

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

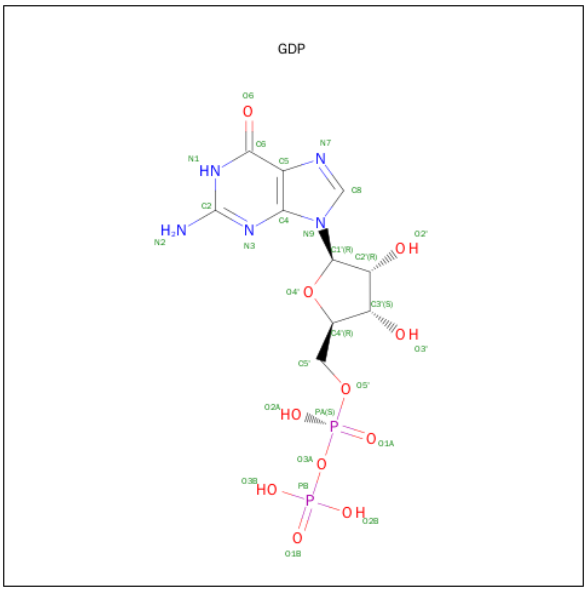
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mg	0	0
			1	1		

- Molecule 3 is TETRAFLUOROALUMINATE ION (three-letter code: ALF) (formula: AlF_4).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	Al	F			
3	A	1	5	1	4		0	0

- Molecule 4 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
4	A	1	28	10	5	11	2	0	0

- Molecule 5 is water.

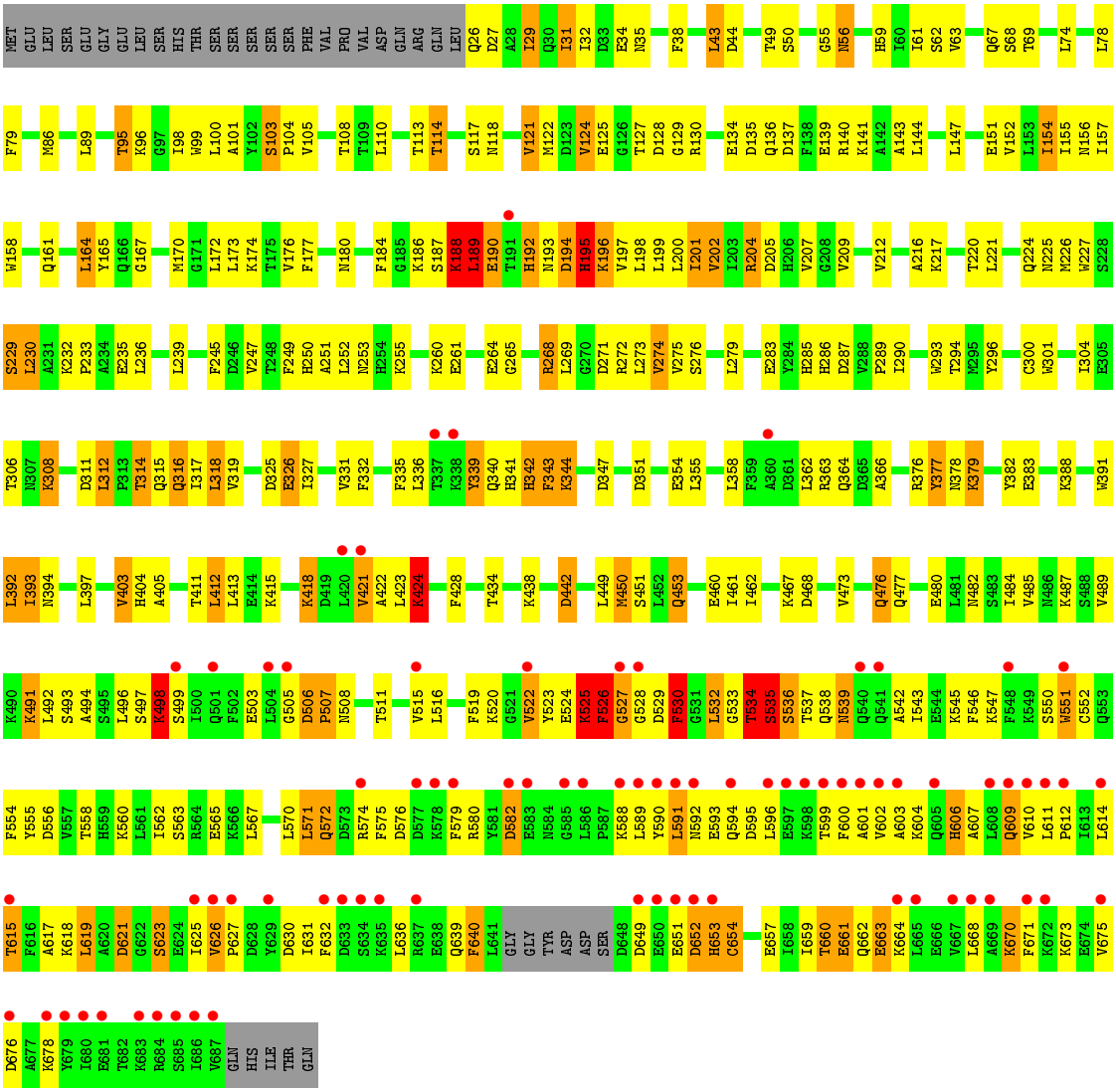
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	115	Total	O	0	0
			115	115		

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: Protein SEY1

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	76.27Å 120.53Å 190.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.76 – 2.80 48.76 – 2.80	Depositor EDS
% Data completeness (in resolution range)	98.9 (48.76-2.80) 99.0 (48.76-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.61 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.253 , 0.279 0.267 , 0.292	Depositor DCC
R_{free} test set	1121 reflections (5.43%)	DCC
Wilson B-factor (Å^2)	64.6	Xtriage
Anisotropy	0.379	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 84.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 21771 reflections	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	5452	wwPDB-VP
Average B, all atoms (Å^2)	91.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.29% 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: GDP, ALF, 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	0.76	1/5404 (0.0%)	1.00	25/7301 (0.3%)

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	A	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	56	ASN	N-CA	-5.29	1.35	1.46

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	661	GLU	CB-CA-C	11.90	134.21	110.40
1	A	424	LYS	N-CA-CB	-10.40	91.88	110.60
1	A	522	VAL	CB-CA-C	-9.88	92.63	111.40
1	A	343	PHE	N-CA-CB	-8.43	95.42	110.60
1	A	421	VAL	CB-CA-C	-8.35	95.53	111.40
1	A	532	LEU	N-CA-C	-7.93	89.58	111.00
1	A	312	LEU	C-N-CD	-7.51	104.07	120.60
1	A	204	ARG	CB-CA-C	-7.51	95.38	110.40
1	A	498	LYS	CB-CA-C	-7.31	95.77	110.40
1	A	196	LYS	N-CA-C	-6.54	93.36	111.00
1	A	194	ASP	CB-CA-C	-6.36	97.67	110.40
1	A	494	ALA	CB-CA-C	-6.33	100.61	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	276	SER	CB-CA-C	6.30	122.08	110.10
1	A	336	LEU	N-CA-C	6.23	127.81	111.00
1	A	527	GLY	N-CA-C	-5.96	98.20	113.10
1	A	526	PHE	N-CA-C	-5.92	95.01	111.00
1	A	532	LEU	CB-CA-C	-5.91	98.98	110.20
1	A	530	PHE	N-CA-C	5.84	126.76	111.00
1	A	651	GLU	CB-CA-C	5.40	121.19	110.40
1	A	453	GLN	N-CA-CB	5.27	120.08	110.60
1	A	525	LYS	N-CA-C	-5.21	96.93	111.00
1	A	393	ILE	CB-CA-C	-5.18	101.25	111.60
1	A	308	LYS	CB-CA-C	-5.10	100.19	110.40
1	A	204	ARG	N-CA-C	5.02	124.56	111.00
1	A	530	PHE	N-CA-CB	-5.01	101.58	110.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	195	HIS	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	5303	0	5245	340	1
2	A	1	0	0	0	0
3	A	5	0	0	1	0
4	A	28	0	12	3	0
5	A	115	0	0	10	0
All	All	5452	0	5257	340	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 32.

All (340) 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:A:193:ASN:HD21	1:A:287:ASP:CB	1.14	1.59
1:A:193:ASN:ND2	1:A:287:ASP:HB2	1.08	1.40
1:A:590:TYR:C	1:A:591:LEU:HD23	1.43	1.38
1:A:193:ASN:ND2	1:A:287:ASP:CB	1.73	1.33
1:A:311:ASP:O	1:A:312:LEU:HD23	1.41	1.20
1:A:192:HIS:HB2	1:A:194:ASP:N	1.55	1.17
1:A:526:PHE:HD2	1:A:546:PHE:CE1	1.68	1.11
1:A:522:VAL:CG1	1:A:522:VAL:O	1.91	1.11
1:A:590:TYR:C	1:A:591:LEU:CD2	2.19	1.10
1:A:192:HIS:HB2	1:A:193:ASN:C	1.73	1.08
1:A:193:ASN:O	1:A:286:HIS:HD2	1.36	1.08
1:A:522:VAL:HG12	1:A:522:VAL:O	1.28	1.08
1:A:188:LYS:O	1:A:190:GLU:CG	2.00	1.07
1:A:424:LYS:HD2	1:A:424:LYS:H	0.91	1.07
1:A:533:GLY:C	1:A:534:THR:HG23	1.74	1.06
1:A:591:LEU:N	1:A:591:LEU:HD23	1.61	1.06
1:A:424:LYS:CD	1:A:424:LYS:H	1.51	1.06
1:A:424:LYS:HD2	1:A:424:LYS:N	1.71	1.06
1:A:533:GLY:O	1:A:534:THR:HG23	1.58	1.04
1:A:188:LYS:HD3	1:A:189:LEU:N	1.73	1.03
1:A:525:LYS:O	1:A:528:GLY:N	1.92	1.01
1:A:418:LYS:O	1:A:421:VAL:HG12	1.61	1.00
1:A:188:LYS:O	1:A:190:GLU:HG3	1.14	0.99
1:A:154:ILE:HD13	1:A:202:VAL:HG13	1.44	0.98
1:A:524:GLU:C	1:A:526:PHE:H	1.50	0.98
1:A:63:VAL:O	1:A:124:VAL:CG1	2.12	0.98
1:A:193:ASN:ND2	1:A:287:ASP:HB3	1.78	0.97
1:A:524:GLU:O	1:A:526:PHE:N	1.98	0.96
1:A:545:LYS:HG2	1:A:640:PHE:HD2	1.31	0.96
1:A:652:ASP:O	1:A:653:HIS:C	2.04	0.96
1:A:190:GLU:O	1:A:192:HIS:CD2	2.19	0.95
1:A:535:SER:HB3	1:A:538:GLN:HB2	1.45	0.95
1:A:450:MET:HG3	1:A:450:MET:O	1.62	0.94
1:A:188:LYS:CD	1:A:189:LEU:N	2.30	0.94
1:A:591:LEU:N	1:A:591:LEU:CD2	2.31	0.94
1:A:530:PHE:CD2	1:A:530:PHE:N	2.35	0.94
1:A:590:TYR:O	1:A:591:LEU:CD2	2.15	0.93
1:A:187:SER:O	1:A:188:LYS:HB2	1.68	0.93
1:A:526:PHE:CD2	1:A:546:PHE:CD1	2.49	0.91
1:A:154:ILE:HD13	1:A:202:VAL:CG1	2.00	0.91
1:A:192:HIS:H	1:A:192:HIS:CD2	1.88	0.90
1:A:526:PHE:CD2	1:A:546:PHE:CZ	2.56	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:524:GLU:C	1:A:526:PHE:N	2.19	0.89
1:A:526:PHE:CD2	1:A:546:PHE:CE1	2.59	0.89
1:A:572:GLN:HA	1:A:575:PHE:HB3	1.56	0.88
1:A:526:PHE:HD2	1:A:546:PHE:CZ	1.81	0.87
1:A:188:LYS:HD3	1:A:188:LYS:C	1.94	0.86
1:A:535:SER:O	1:A:538:GLN:N	2.08	0.86
1:A:525:LYS:O	1:A:527:GLY:CA	2.24	0.85
1:A:530:PHE:H	1:A:530:PHE:HD2	1.24	0.84
1:A:193:ASN:O	1:A:286:HIS:CD2	2.27	0.84
1:A:590:TYR:O	1:A:591:LEU:HD22	1.76	0.84
1:A:520:LYS:HA	1:A:523:TYR:HB3	1.58	0.83
1:A:188:LYS:N	1:A:190:GLU:OE1	2.12	0.83
1:A:193:ASN:HD22	1:A:287:ASP:CB	1.90	0.83
1:A:526:PHE:HD2	1:A:546:PHE:CD1	1.87	0.82
1:A:533:GLY:C	1:A:534:THR:CG2	2.47	0.82
1:A:499:SER:O	1:A:503:GLU:HG2	1.81	0.81
1:A:314:THR:OG1	1:A:316:GLN:N	2.12	0.81
1:A:525:LYS:O	1:A:527:GLY:C	2.20	0.80
1:A:533:GLY:O	1:A:534:THR:CG2	2.30	0.80
1:A:155:ILE:O	1:A:201:ILE:HD12	1.81	0.79
1:A:300:CYS:O	1:A:304:ILE:HG12	1.82	0.79
1:A:582:ASP:HA	1:A:588:LYS:HG3	1.65	0.79
1:A:274:VAL:HG12	1:A:275:VAL:HG23	1.65	0.78
1:A:189:LEU:CD2	1:A:189:LEU:O	2.30	0.78
1:A:534:THR:O	1:A:535:SER:HB2	1.81	0.78
1:A:192:HIS:CB	1:A:193:ASN:C	2.51	0.78
1:A:619:LEU:HD23	1:A:625:ILE:HG12	1.65	0.77
1:A:529:ASP:OD1	1:A:529:ASP:C	2.20	0.77
1:A:63:VAL:HG23	1:A:154:ILE:HG13	1.66	0.77
1:A:235:GLU:HG2	1:A:236:LEU:HG	1.66	0.77
1:A:193:ASN:HD22	1:A:287:ASP:HB3	1.47	0.76
1:A:516:LEU:HA	1:A:519:PHE:HB3	1.65	0.76
1:A:78:LEU:HD22	1:A:269:LEU:HD23	1.68	0.76
1:A:95:THR:N	3:A:702:ALF:F4	2.07	0.76
1:A:144:LEU:HD23	1:A:304:ILE:HD12	1.66	0.76
1:A:421:VAL:CG1	1:A:422:ALA:N	2.48	0.75
1:A:449:LEU:HB2	5:A:803:HOH:O	1.85	0.74
1:A:154:ILE:CD1	1:A:202:VAL:HG13	2.17	0.73
1:A:193:ASN:HD21	1:A:287:ASP:CG	1.91	0.73
1:A:63:VAL:O	1:A:124:VAL:HG13	1.86	0.73
1:A:189:LEU:HD22	1:A:189:LEU:O	1.89	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:476:GLN:HE21	1:A:476:GLN:HA	1.54	0.72
1:A:154:ILE:HD11	1:A:156:ASN:HB2	1.71	0.71
1:A:38:PHE:HB2	1:A:301:TRP:CD1	2.26	0.71
1:A:154:ILE:HA	1:A:200:LEU:O	1.90	0.71
1:A:233:PRO:HG2	1:A:236:LEU:HD12	1.73	0.71
1:A:135:ASP:OD1	1:A:135:ASP:O	2.07	0.71
1:A:55:GLY:O	1:A:289:PRO:HA	1.90	0.71
1:A:507:PRO:HB3	1:A:610:VAL:HG23	1.71	0.70
1:A:563:SER:O	1:A:567:LEU:HB2	1.91	0.70
1:A:190:GLU:O	1:A:192:HIS:HD2	1.74	0.70
1:A:315:GLN:O	1:A:319:VAL:HG23	1.91	0.69
1:A:422:ALA:O	1:A:423:LEU:HD12	1.92	0.69
1:A:194:ASP:OD2	1:A:195:HIS:C	2.29	0.69
1:A:523:TYR:O	1:A:523:TYR:CD1	2.46	0.69
1:A:79:PHE:HB3	1:A:103:SER:HB2	1.75	0.68
1:A:589:LEU:HD23	1:A:591:LEU:HD21	1.75	0.68
1:A:525:LYS:O	1:A:527:GLY:N	2.27	0.68
1:A:63:VAL:HG23	1:A:154:ILE:CG1	2.24	0.68
1:A:534:THR:O	1:A:535:SER:CB	2.41	0.67
1:A:631:ILE:HG22	1:A:632:PHE:H	1.57	0.67
1:A:38:PHE:HB2	1:A:301:TRP:HD1	1.59	0.67
1:A:108:THR:HB	1:A:271:ASP:OD1	1.95	0.67
1:A:499:SER:O	1:A:503:GLU:CG	2.42	0.67
1:A:157:ILE:HG12	1:A:201:ILE:HD11	1.75	0.66
1:A:188:LYS:CD	1:A:189:LEU:H	2.08	0.66
1:A:421:VAL:HG13	1:A:422:ALA:N	2.08	0.66
1:A:193:ASN:HD21	1:A:287:ASP:HB2	0.49	0.65
1:A:626:VAL:HG12	1:A:627:PRO:HD2	1.78	0.65
1:A:662:GLN:OE1	1:A:662:GLN:N	2.29	0.65
1:A:388:LYS:O	1:A:392:LEU:HD12	1.95	0.65
1:A:189:LEU:HD23	1:A:189:LEU:O	1.95	0.65
1:A:192:HIS:CB	1:A:194:ASP:N	2.49	0.65
1:A:193:ASN:O	1:A:286:HIS:HA	1.97	0.65
1:A:545:LYS:HG2	1:A:640:PHE:CD2	2.23	0.65
1:A:192:HIS:HB2	1:A:194:ASP:CA	2.26	0.65
1:A:194:ASP:OD2	1:A:196:LYS:N	2.30	0.65
1:A:311:ASP:O	1:A:312:LEU:CD2	2.33	0.64
1:A:377:TYR:CD1	1:A:377:TYR:N	2.62	0.64
1:A:68:SER:HB3	1:A:86:MET:HE3	1.80	0.64
1:A:534:THR:OG1	1:A:535:SER:N	2.29	0.64
1:A:68:SER:HB3	1:A:86:MET:CE	2.28	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:376:ARG:HB2	1:A:377:TYR:CD1	2.33	0.63
1:A:535:SER:HB3	1:A:538:GLN:CB	2.26	0.63
1:A:156:ASN:HD21	1:A:204:ARG:HH11	1.45	0.63
1:A:193:ASN:OD1	1:A:285:HIS:O	2.16	0.63
1:A:227:TRP:O	1:A:230:LEU:HD12	1.99	0.63
1:A:670:LYS:NZ	5:A:802:HOH:O	2.32	0.63
1:A:551:TRP:CE3	1:A:627:PRO:HA	2.34	0.63
1:A:525:LYS:O	1:A:526:PHE:C	2.37	0.62
1:A:56:ASN:ND2	1:A:287:ASP:OD1	2.28	0.62
1:A:188:LYS:C	1:A:190:GLU:HG3	2.11	0.62
1:A:551:TRP:CZ3	1:A:627:PRO:HA	2.33	0.62
1:A:377:TYR:H	1:A:377:TYR:HD1	1.47	0.62
1:A:192:HIS:C	1:A:194:ASP:H	2.02	0.62
1:A:529:ASP:OD1	1:A:529:ASP:O	2.16	0.62
1:A:449:LEU:N	5:A:803:HOH:O	2.32	0.62
1:A:165:TYR:O	1:A:170:MET:HB2	2.00	0.62
1:A:144:LEU:HD23	1:A:304:ILE:HG23	1.82	0.62
1:A:428:PHE:HB3	1:A:532:LEU:HA	1.82	0.62
1:A:660:THR:OG1	1:A:661:GLU:N	2.30	0.61
1:A:533:GLY:O	1:A:534:THR:CB	2.46	0.61
1:A:535:SER:O	1:A:536:SER:C	2.36	0.61
1:A:562:ILE:HG23	1:A:567:LEU:HD13	1.80	0.61
1:A:311:ASP:C	1:A:312:LEU:HD23	2.17	0.61
1:A:438:LYS:O	1:A:442:ASP:HB2	2.01	0.61
1:A:554:PHE:O	1:A:558:THR:HG23	2.01	0.61
1:A:507:PRO:HB3	1:A:610:VAL:CG2	2.31	0.60
1:A:619:LEU:HD23	1:A:625:ILE:CG1	2.30	0.60
1:A:588:LYS:HE2	1:A:599:THR:HG21	1.84	0.60
1:A:144:LEU:CD2	1:A:304:ILE:HD12	2.30	0.60
1:A:27:ASP:HB2	5:A:859:HOH:O	2.02	0.59
1:A:671:PHE:O	1:A:675:VAL:HB	2.02	0.59
1:A:547:LYS:O	1:A:551:TRP:HD1	1.85	0.59
1:A:157:ILE:CD1	1:A:201:ILE:HD11	2.32	0.59
1:A:428:PHE:HE2	1:A:477:GLN:HG2	1.68	0.59
1:A:476:GLN:NE2	1:A:476:GLN:HA	2.17	0.59
1:A:450:MET:CG	1:A:450:MET:O	2.39	0.59
1:A:571:LEU:HB2	1:A:572:GLN:OE1	2.02	0.58
1:A:473:VAL:O	1:A:477:GLN:HG3	2.03	0.58
1:A:193:ASN:CG	1:A:287:ASP:HB2	2.10	0.58
1:A:147:LEU:HD11	1:A:245:PHE:CE1	2.38	0.58
1:A:619:LEU:HD21	1:A:623:SER:O	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:314:THR:HG23	1:A:317:ILE:HG12	1.84	0.58
1:A:673:LYS:HB2	5:A:813:HOH:O	2.03	0.58
1:A:250:HIS:CD2	1:A:269:LEU:HB2	2.39	0.58
1:A:619:LEU:HD12	1:A:621:ASP:HB2	1.86	0.58
1:A:574:ARG:HH22	1:A:609:GLN:HG3	1.69	0.58
1:A:673:LYS:CB	5:A:813:HOH:O	2.52	0.57
1:A:403:VAL:HG12	1:A:404:HIS:N	2.19	0.57
1:A:68:SER:CB	1:A:86:MET:CE	2.83	0.57
1:A:652:ASP:O	1:A:654:CYS:N	2.38	0.57
1:A:326:GLU:HG2	1:A:327:ILE:N	2.19	0.57
1:A:253:ASN:OD1	1:A:261:GLU:HB3	2.05	0.57
1:A:67:GLN:OE1	1:A:129:GLY:HA3	2.04	0.56
1:A:424:LYS:CD	1:A:424:LYS:N	2.32	0.56
1:A:314:THR:OG1	1:A:315:GLN:N	2.36	0.56
1:A:157:ILE:CG1	1:A:201:ILE:HD11	2.35	0.56
1:A:391:TRP:HA	1:A:394:ASN:HB2	1.87	0.56
1:A:192:HIS:C	1:A:194:ASP:N	2.60	0.55
1:A:377:TYR:HD1	1:A:377:TYR:N	2.05	0.55
1:A:188:LYS:HD2	1:A:189:LEU:N	2.19	0.55
1:A:498:LYS:HG2	1:A:499:SER:N	2.10	0.55
1:A:603:ALA:O	1:A:607:ALA:N	2.40	0.55
1:A:339:TYR:C	1:A:341:HIS:H	2.10	0.54
1:A:127:THR:O	1:A:128:ASP:HB3	2.05	0.54
1:A:216:ALA:O	1:A:220:THR:HG23	2.07	0.54
1:A:127:THR:O	1:A:128:ASP:CB	2.55	0.54
1:A:177:PHE:O	1:A:180:ASN:HB3	2.08	0.54
1:A:592:ASN:HB3	1:A:594:GLN:HB2	1.90	0.54
1:A:155:ILE:HG22	1:A:201:ILE:HD13	1.90	0.54
1:A:161:GLN:HA	1:A:164:LEU:HD22	1.89	0.54
1:A:29:ILE:H	1:A:29:ILE:HD12	1.72	0.54
1:A:265:GLY:HA2	1:A:268:ARG:NH1	2.24	0.53
1:A:536:SER:HA	1:A:539:ASN:HB2	1.91	0.53
1:A:593:GLU:HA	1:A:596:LEU:HB3	1.90	0.53
1:A:492:LEU:O	1:A:496:LEU:HB2	2.09	0.53
1:A:140:ARG:HA	1:A:172:LEU:HD11	1.90	0.53
1:A:68:SER:OG	1:A:86:MET:CE	2.57	0.52
1:A:602:VAL:O	1:A:606:HIS:HB2	2.09	0.52
1:A:508:ASN:H	1:A:511:THR:HG23	1.73	0.52
1:A:205:ASP:OD2	4:A:703:GDP:N2	2.35	0.52
1:A:212:VAL:CG2	1:A:251:ALA:HB2	2.39	0.52
1:A:192:HIS:N	1:A:192:HIS:CD2	2.67	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:507:PRO:CB	1:A:610:VAL:HG23	2.40	0.52
1:A:296:TYR:O	1:A:300:CYS:SG	2.68	0.51
1:A:619:LEU:CD1	1:A:621:ASP:HB2	2.39	0.51
1:A:543:ILE:HG22	1:A:547:LYS:HG3	1.93	0.51
1:A:505:GLY:O	1:A:506:ASP:HB2	2.10	0.51
1:A:535:SER:O	1:A:537:THR:N	2.44	0.50
1:A:449:LEU:CA	5:A:803:HOH:O	2.59	0.50
1:A:139:GLU:OE2	1:A:172:LEU:HD22	2.11	0.50
1:A:611:LEU:HB2	1:A:612:PRO:HD3	1.92	0.50
1:A:533:GLY:O	1:A:534:THR:OG1	2.29	0.50
1:A:250:HIS:NE2	1:A:269:LEU:HB2	2.27	0.50
1:A:351:ASP:HB3	1:A:354:GLU:HB2	1.93	0.50
1:A:589:LEU:HD23	1:A:591:LEU:CD2	2.41	0.50
1:A:154:ILE:HD12	1:A:154:ILE:C	2.33	0.50
1:A:113:THR:HG22	1:A:114:THR:O	2.12	0.49
1:A:161:GLN:NE2	1:A:167:GLY:O	2.27	0.49
1:A:187:SER:OG	1:A:187:SER:O	2.30	0.49
1:A:489:VAL:HG12	1:A:489:VAL:O	2.11	0.49
1:A:519:PHE:O	1:A:523:TYR:HB2	2.13	0.49
1:A:342:HIS:HD2	1:A:358:LEU:HD11	1.77	0.49
1:A:676:ASP:C	1:A:678:LYS:H	2.14	0.49
1:A:575:PHE:HE1	1:A:675:VAL:HG13	1.78	0.49
1:A:523:TYR:HH	1:A:551:TRP:HE1	1.59	0.48
1:A:526:PHE:C	1:A:526:PHE:HD1	2.17	0.48
1:A:376:ARG:HB2	1:A:377:TYR:CE1	2.48	0.48
1:A:59:HIS:HD2	1:A:151:GLU:OE2	1.96	0.48
1:A:525:LYS:O	1:A:527:GLY:HA2	2.07	0.48
1:A:212:VAL:HG22	1:A:251:ALA:HB2	1.95	0.48
1:A:50:SER:OG	1:A:118:ASN:ND2	2.47	0.48
1:A:29:ILE:N	1:A:29:ILE:HD12	2.29	0.48
1:A:575:PHE:CE1	1:A:675:VAL:HG13	2.49	0.48
1:A:68:SER:CB	1:A:86:MET:HE1	2.44	0.48
1:A:659:ILE:HG13	1:A:663:GLU:HB2	1.96	0.48
1:A:524:GLU:O	1:A:525:LYS:C	2.51	0.47
1:A:63:VAL:O	1:A:124:VAL:HG11	2.08	0.47
1:A:141:LYS:HG2	1:A:304:ILE:HG22	1.97	0.47
1:A:136:GLN:O	1:A:140:ARG:HG3	2.13	0.47
1:A:601:ALA:HA	1:A:604:LYS:HG3	1.95	0.47
1:A:99:TRP:O	1:A:122:MET:HA	2.15	0.47
1:A:528:GLY:C	1:A:529:ASP:O	2.49	0.47
1:A:332:PHE:O	1:A:335:PHE:N	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:157:ILE:HD11	1:A:201:ILE:HD11	1.97	0.47
1:A:100:LEU:HD12	1:A:122:MET:HG3	1.97	0.47
1:A:522:VAL:HG13	1:A:522:VAL:O	2.05	0.47
1:A:343:PHE:O	1:A:344:LYS:C	2.51	0.47
1:A:619:LEU:CD2	1:A:625:ILE:HG12	2.40	0.46
1:A:101:ALA:O	1:A:121:VAL:HG13	2.15	0.46
1:A:61:ILE:HG23	1:A:61:ILE:O	2.15	0.46
1:A:428:PHE:CB	1:A:532:LEU:HA	2.46	0.46
1:A:147:LEU:HD11	1:A:245:PHE:HE1	1.80	0.46
1:A:450:MET:N	5:A:803:HOH:O	2.48	0.46
1:A:379:LYS:O	1:A:383:GLU:N	2.45	0.46
1:A:225:ASN:O	1:A:226:MET:C	2.53	0.45
1:A:377:TYR:O	1:A:378:ASN:C	2.52	0.45
1:A:335:PHE:CZ	1:A:393:ILE:HG23	2.52	0.45
1:A:428:PHE:CE2	1:A:477:GLN:HG2	2.48	0.45
1:A:351:ASP:HB3	1:A:354:GLU:CD	2.37	0.45
1:A:652:ASP:O	1:A:653:HIS:O	2.33	0.45
1:A:174:LYS:HD2	1:A:229:SER:OG	2.17	0.45
1:A:34:GLU:HG3	1:A:96:LYS:HB3	1.98	0.45
1:A:582:ASP:CA	1:A:588:LYS:HG3	2.41	0.44
1:A:62:SER:HB3	1:A:122:MET:HB2	1.99	0.44
1:A:379:LYS:HE2	1:A:379:LYS:HB3	1.73	0.44
1:A:526:PHE:C	1:A:526:PHE:CD1	2.91	0.44
1:A:631:ILE:O	1:A:632:PHE:HB2	2.17	0.44
1:A:100:LEU:HD12	1:A:122:MET:CG	2.47	0.44
1:A:199:LEU:HB2	1:A:247:VAL:HG12	1.99	0.44
1:A:619:LEU:C	1:A:621:ASP:H	2.21	0.44
1:A:339:TYR:C	1:A:341:HIS:N	2.71	0.44
1:A:43:LEU:HG	1:A:294:THR:HG21	2.00	0.44
1:A:485:VAL:HG22	1:A:542:ALA:O	2.17	0.44
1:A:49:THR:OG1	1:A:50:SER:N	2.50	0.44
1:A:421:VAL:HG12	1:A:422:ALA:N	2.29	0.44
1:A:306:THR:HG23	1:A:306:THR:O	2.17	0.44
1:A:555:TYR:HH	1:A:632:PHE:HZ	1.61	0.44
1:A:393:ILE:O	1:A:393:ILE:CG2	2.64	0.44
1:A:331:VAL:HG12	1:A:366:ALA:HB1	1.99	0.44
1:A:312:LEU:HA	1:A:312:LEU:HD23	1.66	0.43
1:A:143:ALA:HB3	1:A:176:VAL:HG21	2.00	0.43
1:A:522:VAL:C	1:A:524:GLU:H	2.18	0.43
1:A:331:VAL:CG1	1:A:366:ALA:HB1	2.48	0.43
1:A:491:LYS:HA	1:A:491:LYS:HD3	1.56	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:317:ILE:O	1:A:318:LEU:C	2.56	0.43
1:A:393:ILE:O	1:A:393:ILE:HG22	2.16	0.43
1:A:611:LEU:HB3	1:A:615:THR:HG23	1.99	0.43
1:A:424:LYS:HA	1:A:480:GLU:OE1	2.19	0.43
1:A:378:ASN:O	1:A:382:TYR:HB3	2.19	0.42
1:A:654:CYS:HB3	1:A:657:GLU:HB2	2.00	0.42
1:A:673:LYS:HB3	5:A:813:HOH:O	2.18	0.42
1:A:283:GLU:H	1:A:283:GLU:CD	2.21	0.42
1:A:63:VAL:O	1:A:124:VAL:HG12	2.11	0.42
1:A:61:ILE:CD1	1:A:152:VAL:HB	2.50	0.42
1:A:411:THR:HG22	1:A:412:LEU:N	2.34	0.42
1:A:404:HIS:O	1:A:405:ALA:C	2.55	0.42
1:A:187:SER:O	1:A:188:LYS:CB	2.46	0.42
1:A:418:LYS:HZ2	1:A:421:VAL:HG11	1.84	0.42
1:A:61:ILE:HG23	1:A:121:VAL:HA	2.00	0.42
1:A:579:PHE:CE1	1:A:600:PHE:HA	2.54	0.42
1:A:639:GLN:HB2	1:A:640:PHE:CE1	2.55	0.42
1:A:134:GLU:HG2	1:A:314:THR:HB	2.01	0.42
1:A:335:PHE:CE1	1:A:393:ILE:HG23	2.55	0.42
1:A:226:MET:O	1:A:226:MET:HG2	2.20	0.42
1:A:31:ILE:HD11	1:A:98:ILE:HG22	2.01	0.42
1:A:69:THR:HA	1:A:158:TRP:CZ2	2.55	0.42
1:A:364:GLN:NE2	1:A:364:GLN:O	2.53	0.42
1:A:61:ILE:HD12	1:A:152:VAL:HB	2.02	0.41
1:A:152:VAL:HG22	1:A:198:LEU:HB3	2.02	0.41
1:A:260:LYS:O	1:A:264:GLU:HG3	2.20	0.41
1:A:550:SER:C	1:A:552:CYS:H	2.23	0.41
1:A:467:LYS:HG3	1:A:468:ASP:N	2.35	0.41
1:A:424:LYS:HG2	1:A:424:LYS:O	2.20	0.41
1:A:188:LYS:HD2	1:A:189:LEU:H	1.80	0.41
1:A:422:ALA:C	1:A:423:LEU:HD12	2.39	0.41
1:A:325:ASP:O	1:A:326:GLU:C	2.58	0.41
1:A:515:VAL:HG12	1:A:516:LEU:HD12	2.01	0.41
1:A:136:GLN:O	1:A:137:ASP:C	2.59	0.41
1:A:201:ILE:HG12	1:A:249:PHE:CE1	2.56	0.41
1:A:523:TYR:CG	1:A:523:TYR:O	2.73	0.41
1:A:498:LYS:HG2	1:A:498:LYS:O	2.04	0.41
1:A:507:PRO:CB	1:A:610:VAL:CG2	2.98	0.41
1:A:659:ILE:HG23	1:A:659:ILE:O	2.21	0.40
1:A:155:ILE:O	1:A:201:ILE:CD1	2.61	0.40
1:A:232:LYS:HA	1:A:233:PRO:HD2	1.94	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:546:PHE:C	1:A:546:PHE:CD1	2.94	0.40
1:A:255:LYS:HD3	4:A:703:GDP:C5	2.57	0.40
1:A:290:ILE:O	1:A:294:THR:HG23	2.21	0.40
1:A:293:TRP:O	1:A:294:THR:C	2.59	0.40
1:A:412:LEU:O	1:A:413:LEU:C	2.60	0.40
1:A:339:TYR:O	1:A:343:PHE:HB2	2.22	0.40
1:A:205:ASP:CG	4:A:703:GDP:HN1	2.20	0.40
1:A:212:VAL:HG21	1:A:251:ALA:HB2	2.04	0.40
1:A:489:VAL:O	1:A:489:VAL:CG1	2.69	0.40
1:A:393:ILE:O	1:A:397:LEU:HG	2.21	0.40
1:A:579:PHE:HD2	5:A:816:HOH:O	2.04	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:224:GLN:OE1	1:A:453:GLN:NE2[4_555]	2.00	0.20

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	652/692 (94%)	543 (83%)	92 (14%)	17 (3%)	7 22

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	188	LYS
1	A	189	LEU
1	A	506	ASP
1	A	534	THR
1	A	535	SER

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Mol	Chain	Res	Type
1	A	536	SER
1	A	660	THR
1	A	663	GLU
1	A	617	ALA
1	A	652	ASP
1	A	653	HIS
1	A	525	LYS
1	A	551	TRP
1	A	582	ASP
1	A	507	PRO
1	A	104	PRO
1	A	403	VAL

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	588/621 (95%)	475 (81%)	113 (19%)	2 5

All (113) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	GLN
1	A	29	ILE
1	A	31	ILE
1	A	32	ILE
1	A	35	ASN
1	A	43	LEU
1	A	44	ASP
1	A	74	LEU
1	A	89	LEU
1	A	95	THR
1	A	103	SER
1	A	105	VAL
1	A	110	LEU
1	A	114	THR

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Mol	Chain	Res	Type
1	A	117	SER
1	A	121	VAL
1	A	124	VAL
1	A	125	GLU
1	A	130	ARG
1	A	154	ILE
1	A	164	LEU
1	A	173	LEU
1	A	184	PHE
1	A	186	LYS
1	A	188	LYS
1	A	189	LEU
1	A	190	GLU
1	A	192	HIS
1	A	195	HIS
1	A	197	VAL
1	A	201	ILE
1	A	202	VAL
1	A	207	VAL
1	A	209	VAL
1	A	217	LYS
1	A	221	LEU
1	A	229	SER
1	A	230	LEU
1	A	239	LEU
1	A	252	LEU
1	A	268	ARG
1	A	272	ARG
1	A	273	LEU
1	A	274	VAL
1	A	279	LEU
1	A	308	LYS
1	A	314	THR
1	A	316	GLN
1	A	318	LEU
1	A	326	GLU
1	A	339	TYR
1	A	340	GLN
1	A	342	HIS
1	A	344	LYS
1	A	347	ASP
1	A	355	LEU

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Mol	Chain	Res	Type
1	A	362	LEU
1	A	363	ARG
1	A	377	TYR
1	A	379	LYS
1	A	392	LEU
1	A	412	LEU
1	A	415	LYS
1	A	418	LYS
1	A	424	LYS
1	A	434	THR
1	A	442	ASP
1	A	450	MET
1	A	451	SER
1	A	460	GLU
1	A	461	ILE
1	A	462	ILE
1	A	476	GLN
1	A	482	ASN
1	A	484	ILE
1	A	487	LYS
1	A	491	LYS
1	A	493	SER
1	A	497	SER
1	A	498	LYS
1	A	525	LYS
1	A	526	PHE
1	A	530	PHE
1	A	534	THR
1	A	535	SER
1	A	539	ASN
1	A	556	ASP
1	A	560	LYS
1	A	565	GLU
1	A	570	LEU
1	A	571	LEU
1	A	572	GLN
1	A	576	ASP
1	A	580	ARG
1	A	591	LEU
1	A	595	ASP
1	A	606	HIS
1	A	609	GLN

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Mol	Chain	Res	Type
1	A	614	LEU
1	A	615	THR
1	A	618	LYS
1	A	619	LEU
1	A	621	ASP
1	A	623	SER
1	A	626	VAL
1	A	630	ASP
1	A	636	LEU
1	A	640	PHE
1	A	649	ASP
1	A	654	CYS
1	A	664	LYS
1	A	668	LEU
1	A	670	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	59	HIS
1	A	118	ASN
1	A	156	ASN
1	A	166	GLN
1	A	192	HIS
1	A	193	ASN
1	A	206	HIS
1	A	238	HIS
1	A	285	HIS
1	A	286	HIS
1	A	315	GLN
1	A	316	GLN
1	A	340	GLN
1	A	476	GLN
1	A	482	ASN
1	A	501	GLN
1	A	514	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 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	$\#\|Z\| > 2$
3	ALF	A	702	-	0,4,4	0.00	-	0,6,6	0.00	-
4	GDP	A	703	2	24,30,30	1.54	3 (12%)	26,47,47	2.07	8 (30%)

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
3	ALF	A	702	-	-	0/0/0/0	0/0/0/0
4	GDP	A	703	2	-	0/12/32/32	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	703	GDP	C2'-C1'	-4.44	1.46	1.53
4	A	703	GDP	C8-N7	2.04	1.38	1.34
4	A	703	GDP	C5-C4	3.49	1.48	1.40

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	703	GDP	C5-C6-N1	-4.27	117.94	123.52
4	A	703	GDP	O5'-PA-O1A	-4.13	92.29	109.21
4	A	703	GDP	N3-C2-N1	-2.27	124.47	127.56
4	A	703	GDP	O4'-C1'-N9	-2.12	104.09	108.11
4	A	703	GDP	O3'-C3'-C2'	-2.09	105.11	111.86
4	A	703	GDP	O3B-PB-O2B	2.35	116.08	107.44
4	A	703	GDP	O2A-PA-O3A	3.51	120.31	105.27
4	A	703	GDP	C6-N1-C2	4.34	120.97	115.88

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	702	ALF	1	0
4	A	703	GDP	3	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, 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	656/692 (94%)	0.60	80 (12%) 5 3	33, 77, 188, 281	0

All (80) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	680	ILE	28.9
1	A	679	TYR	12.6
1	A	598	LYS	9.6
1	A	578	LYS	9.3
1	A	668	LEU	8.9
1	A	590	TYR	8.6
1	A	603	ALA	8.2
1	A	665	LEU	8.2
1	A	605	GLN	8.0
1	A	612	PRO	7.5
1	A	672	LYS	7.2
1	A	596	LEU	7.0
1	A	582	ASP	7.0
1	A	579	PHE	6.9
1	A	601	ALA	6.7
1	A	683	LYS	6.7
1	A	599	THR	6.3
1	A	614	LEU	6.2
1	A	577	ASP	6.1
1	A	583	GLU	5.7
1	A	650	GLU	5.5
1	A	589	LEU	5.4
1	A	592	ASN	5.4
1	A	627	PRO	5.1
1	A	594	GLN	4.9
1	A	191	THR	4.9
1	A	602	VAL	4.8

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Mol	Chain	Res	Type	RSRZ
1	A	653	HIS	4.7
1	A	591	LEU	4.7
1	A	551	TRP	4.7
1	A	649	ASP	4.6
1	A	685	SER	4.6
1	A	676	ASP	4.4
1	A	669	ALA	4.3
1	A	667	VAL	4.3
1	A	600	PHE	4.3
1	A	634	SER	4.0
1	A	338	LYS	3.8
1	A	675	VAL	3.8
1	A	541	GLN	3.8
1	A	684	ARG	3.7
1	A	651	GLU	3.7
1	A	499	SER	3.5
1	A	610	VAL	3.5
1	A	608	LEU	3.5
1	A	633	ASP	3.4
1	A	609	GLN	3.4
1	A	629	TYR	3.3
1	A	686	ILE	3.3
1	A	664	LYS	3.2
1	A	625	ILE	3.2
1	A	652	ASP	3.1
1	A	635	LYS	3.0
1	A	632	PHE	2.9
1	A	626	VAL	2.9
1	A	585	GLY	2.8
1	A	678	LYS	2.8
1	A	671	PHE	2.8
1	A	522	VAL	2.8
1	A	615	THR	2.8
1	A	515	VAL	2.7
1	A	681	GLU	2.7
1	A	586	LEU	2.7
1	A	637	ARG	2.7
1	A	548	PHE	2.6
1	A	505	GLY	2.6
1	A	574	ARG	2.6
1	A	528	GLY	2.6
1	A	337	THR	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	420	LEU	2.5
1	A	588	LYS	2.5
1	A	540	GLN	2.4
1	A	504	LEU	2.4
1	A	360	ALA	2.3
1	A	421	VAL	2.2
1	A	687	VAL	2.2
1	A	527	GLY	2.1
1	A	501	GLN	2.1
1	A	597	GLU	2.1
1	A	611	LEU	2.1

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	ALF	A	702	5/5	0.98	0.27	1.67	31,32,40,41	0
4	GDP	A	703	28/28	0.98	0.24	0.59	22,29,38,42	0
2	MG	A	701	1/1	0.94	0.25	-	30,30,30,30	0

6.5 Other polymers (i)

There are no such residues in this entry.