Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 06:16 pm BST

PDB ID	:	6G1F
Title	:	Crystal structure of D-phenylglycine aninotransferase (D-PhgAT) from Pseudomonas stutzeri with PLP internal aldimine
Authors	:	Serpico, A.; Marles-Wright, J.; Campopiano, D.J.
Deposited on	:	2018-03-21
Resolution	:	2.25 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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

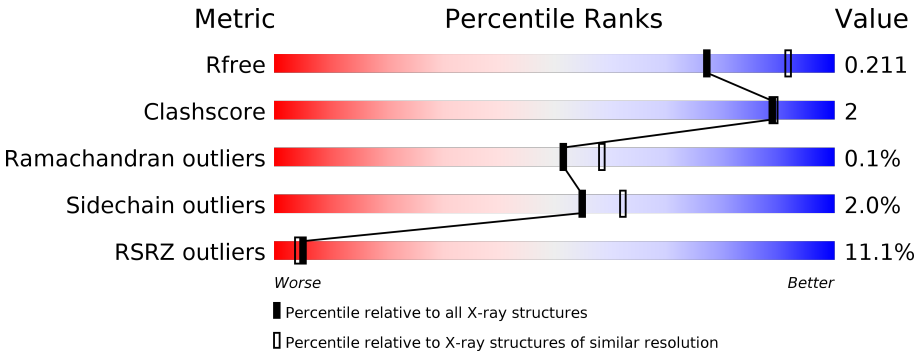
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 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}	130704	2391 (2.26-2.22)
Clashscore	141614	2539 (2.26-2.22)
Ramachandran outliers	138981	2489 (2.26-2.22)
Sidechain outliers	138945	2490 (2.26-2.22)
RSRZ outliers	127900	2353 (2.26-2.22)

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 respectively. 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	464	9% 91% 5% 5%
1	B	464	5% 88% 6% 5%
1	C	464	11% 89% 6% 5%
1	D	464	8% 90% 5% 5%
1	E	464	12% 88% 5% • 6%
1	F	464	19% 88% 6% 6%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 40487 atoms, of which 19845 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 D-phenylglycine aminotransferase.

Mol	Chain	Residues	Atoms							ZeroOcc	AltConf	Trace
1	A	443	Total	C	H	N	O	P	S	0	0	0
			6726	2141	3329	618	625	1	12			
1	B	441	Total	C	H	N	O	P	S	0	0	0
			6690	2127	3313	615	622	1	12			
1	C	440	Total	C	H	N	O	P	S	0	0	0
			6683	2125	3310	614	621	1	12			
1	D	441	Total	C	H	N	O	P	S	0	0	0
			6689	2127	3312	615	622	1	12			
1	E	438	Total	C	H	N	O	P	S	0	0	0
			6653	2116	3297	611	616	1	12			
1	F	438	Total	C	H	N	O	P	S	0	0	0
			6637	2111	3284	611	618	1	12			

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-10	MET	-	initiating methionine	UNP Q6VY99
A	-9	SER	-	expression tag	UNP Q6VY99
A	-8	HIS	-	expression tag	UNP Q6VY99
A	-7	HIS	-	expression tag	UNP Q6VY99
A	-6	HIS	-	expression tag	UNP Q6VY99
A	-5	HIS	-	expression tag	UNP Q6VY99
A	-4	HIS	-	expression tag	UNP Q6VY99
A	-3	HIS	-	expression tag	UNP Q6VY99
A	-2	GLY	-	expression tag	UNP Q6VY99
A	-1	SER	-	expression tag	UNP Q6VY99
A	0	SER	-	expression tag	UNP Q6VY99
A	1	GLY	-	expression tag	UNP Q6VY99
B	-10	MET	-	initiating methionine	UNP Q6VY99
B	-9	SER	-	expression tag	UNP Q6VY99
B	-8	HIS	-	expression tag	UNP Q6VY99
B	-7	HIS	-	expression tag	UNP Q6VY99
B	-6	HIS	-	expression tag	UNP Q6VY99

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-5	HIS	-	expression tag	UNP Q6VY99
B	-4	HIS	-	expression tag	UNP Q6VY99
B	-3	HIS	-	expression tag	UNP Q6VY99
B	-2	GLY	-	expression tag	UNP Q6VY99
B	-1	SER	-	expression tag	UNP Q6VY99
B	0	SER	-	expression tag	UNP Q6VY99
B	1	GLY	-	expression tag	UNP Q6VY99
C	-10	MET	-	initiating methionine	UNP Q6VY99
C	-9	SER	-	expression tag	UNP Q6VY99
C	-8	HIS	-	expression tag	UNP Q6VY99
C	-7	HIS	-	expression tag	UNP Q6VY99
C	-6	HIS	-	expression tag	UNP Q6VY99
C	-5	HIS	-	expression tag	UNP Q6VY99
C	-4	HIS	-	expression tag	UNP Q6VY99
C	-3	HIS	-	expression tag	UNP Q6VY99
C	-2	GLY	-	expression tag	UNP Q6VY99
C	-1	SER	-	expression tag	UNP Q6VY99
C	0	SER	-	expression tag	UNP Q6VY99
C	1	GLY	-	expression tag	UNP Q6VY99
D	-10	MET	-	initiating methionine	UNP Q6VY99
D	-9	SER	-	expression tag	UNP Q6VY99
D	-8	HIS	-	expression tag	UNP Q6VY99
D	-7	HIS	-	expression tag	UNP Q6VY99
D	-6	HIS	-	expression tag	UNP Q6VY99
D	-5	HIS	-	expression tag	UNP Q6VY99
D	-4	HIS	-	expression tag	UNP Q6VY99
D	-3	HIS	-	expression tag	UNP Q6VY99
D	-2	GLY	-	expression tag	UNP Q6VY99
D	-1	SER	-	expression tag	UNP Q6VY99
D	0	SER	-	expression tag	UNP Q6VY99
D	1	GLY	-	expression tag	UNP Q6VY99
E	-10	MET	-	initiating methionine	UNP Q6VY99
E	-9	SER	-	expression tag	UNP Q6VY99
E	-8	HIS	-	expression tag	UNP Q6VY99
E	-7	HIS	-	expression tag	UNP Q6VY99
E	-6	HIS	-	expression tag	UNP Q6VY99
E	-5	HIS	-	expression tag	UNP Q6VY99
E	-4	HIS	-	expression tag	UNP Q6VY99
E	-3	HIS	-	expression tag	UNP Q6VY99
E	-2	GLY	-	expression tag	UNP Q6VY99
E	-1	SER	-	expression tag	UNP Q6VY99
E	0	SER	-	expression tag	UNP Q6VY99

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Chain	Residue	Modelled	Actual	Comment	Reference
E	1	GLY	-	expression tag	UNP Q6VY99
F	-10	MET	-	initiating methionine	UNP Q6VY99
F	-9	SER	-	expression tag	UNP Q6VY99
F	-8	HIS	-	expression tag	UNP Q6VY99
F	-7	HIS	-	expression tag	UNP Q6VY99
F	-6	HIS	-	expression tag	UNP Q6VY99
F	-5	HIS	-	expression tag	UNP Q6VY99
F	-4	HIS	-	expression tag	UNP Q6VY99
F	-3	HIS	-	expression tag	UNP Q6VY99
F	-2	GLY	-	expression tag	UNP Q6VY99
F	-1	SER	-	expression tag	UNP Q6VY99
F	0	SER	-	expression tag	UNP Q6VY99
F	1	GLY	-	expression tag	UNP Q6VY99

- Molecule 2 is water.

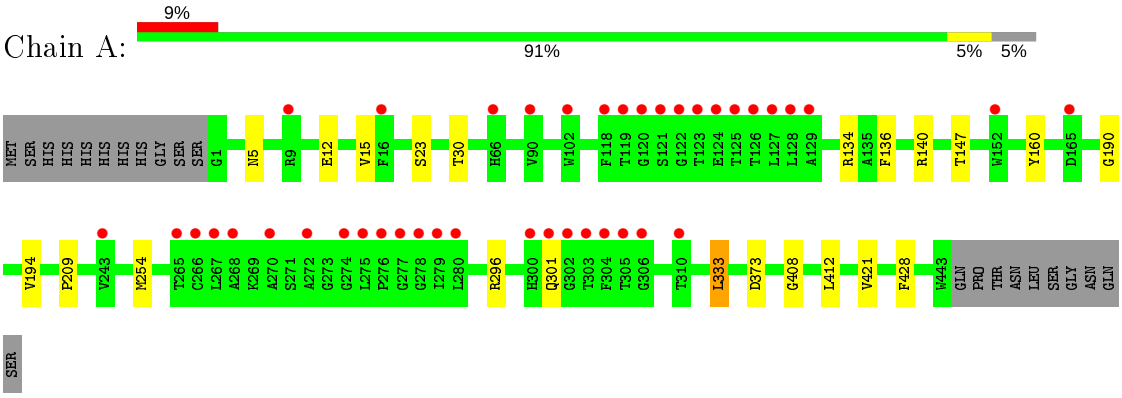
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	106	Total O 106 106	0	0
2	B	120	Total O 120 120	0	0
2	C	59	Total O 59 59	0	0
2	D	83	Total O 83 83	0	0
2	E	35	Total O 35 35	0	0
2	F	6	Total O 6 6	0	0

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 the various outlier classes 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.

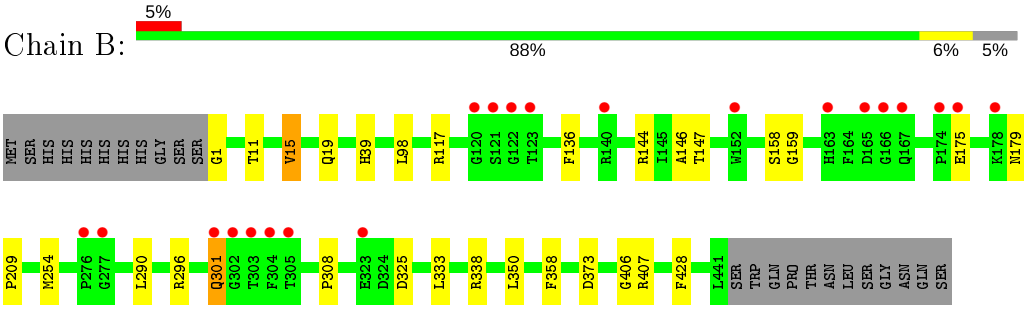
- Molecule 1: D-phenylglycine aminotransferase

Chain A:



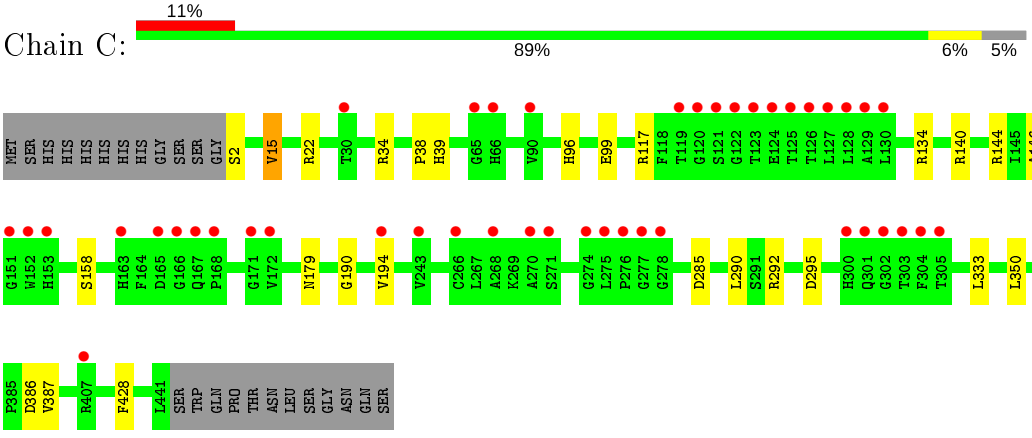
- Molecule 1: D-phenylglycine aminotransferase

Chain B:



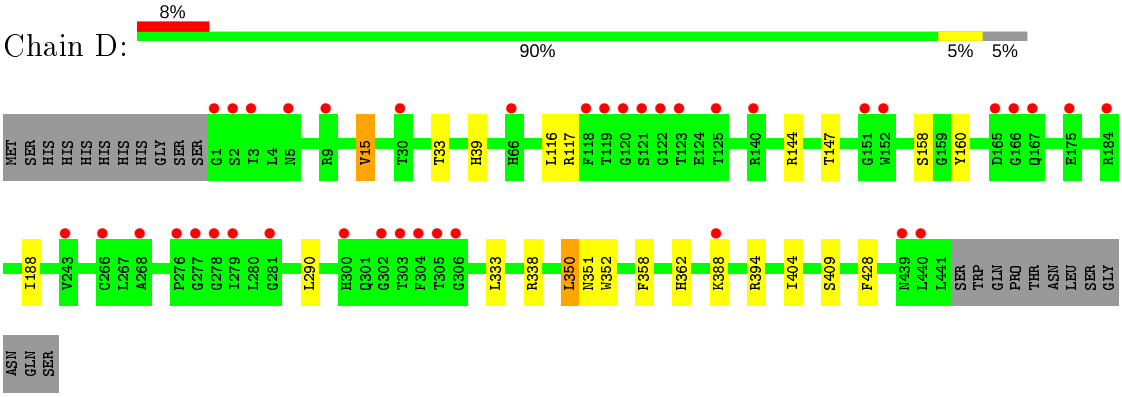
- Molecule 1: D-phenylglycine aminotransferase

Chain C:



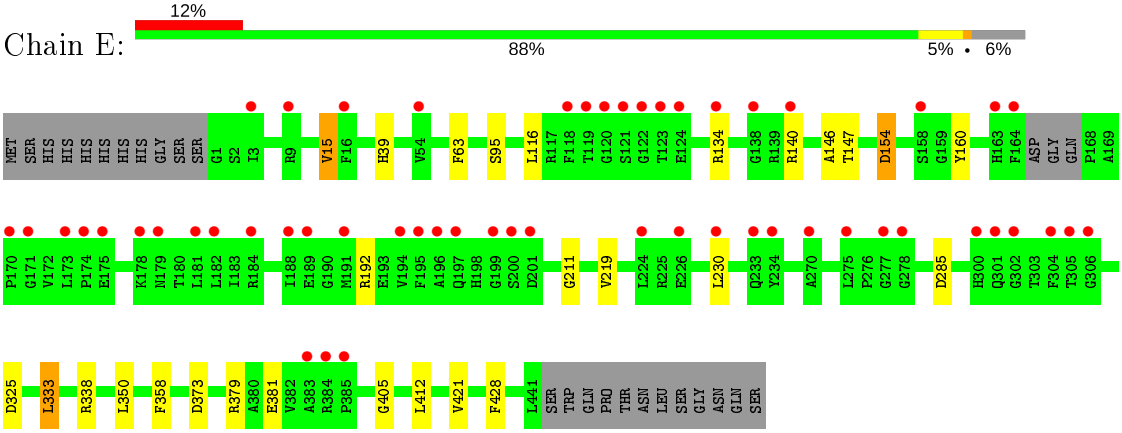
• Molecule 1: D-phenylglycine aminotransferase

Chain D:



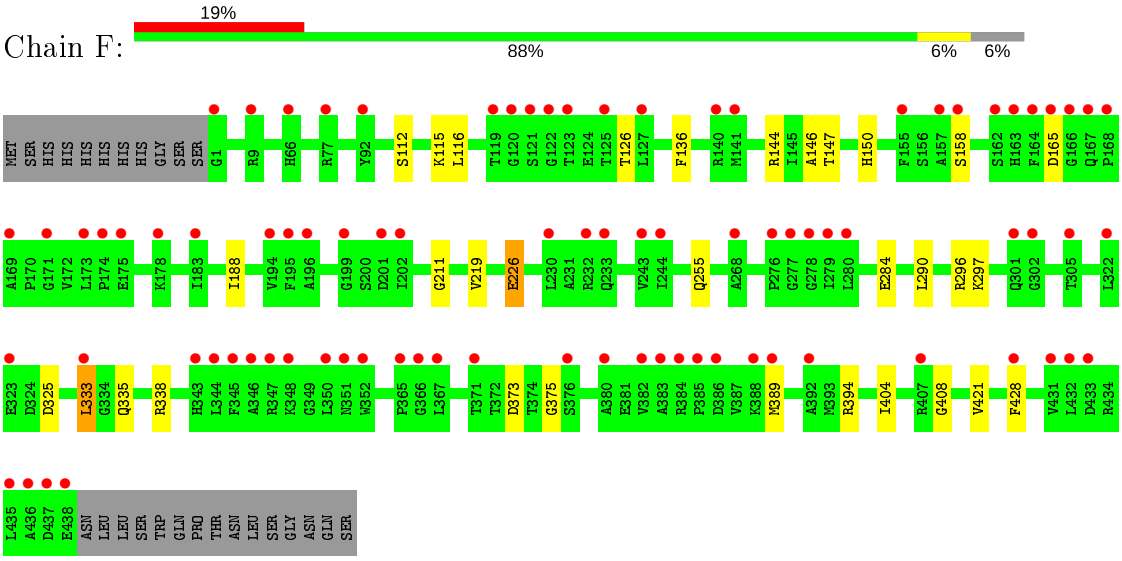
• Molecule 1: D-phenylglycine aminotransferase

Chain E:



• Molecule 1: D-phenylglycine aminotransferase

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	329.28Å 83.90Å 133.42Å 90.00° 111.58° 90.00°	Depositor
Resolution (Å)	49.47 – 2.25 49.46 – 2.25	Depositor EDS
% Data completeness (in resolution range)	99.8 (49.47-2.25) 99.8 (49.46-2.25)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.41 (at 2.25Å)	Xtriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, R_{free}	0.183 , 0.211 0.183 , 0.211	Depositor DCC
R_{free} test set	8147 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å^2)	47.8	Xtriage
Anisotropy	0.261	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.41 , 46.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.006 for -h-2*l,-k,l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	40487	wwPDB-VP
Average B, all atoms (Å^2)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.38% 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: LLP

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	0.27	0/3449	0.45	0/4675
1	B	0.27	0/3427	0.46	0/4644
1	C	0.26	0/3423	0.44	0/4639
1	D	0.26	0/3427	0.45	0/4644
1	E	0.25	0/3405	0.43	0/4612
1	F	0.25	0/3403	0.41	0/4611
All	All	0.26	0/20534	0.44	0/27825

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3397	3329	3329	9	0
1	B	3377	3313	3314	14	0
1	C	3373	3310	3308	14	0
1	D	3377	3312	3314	11	0
1	E	3356	3297	3299	14	0
1	F	3353	3284	3286	15	0
2	A	106	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	120	0	0	1	0
2	C	59	0	0	1	0
2	D	83	0	0	0	0
2	E	35	0	0	0	0
2	F	6	0	0	0	0
All	All	20642	19845	19850	74	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 2.

All (74) 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:E:146:ALA:O	1:E:147:THR:OG1	1.99	0.78
1:D:338:ARG:NH2	1:D:358:PHE:O	2.18	0.76
1:E:134:ARG:NH1	1:E:140:ARG:O	2.22	0.72
1:C:146:ALA:O	1:C:147:THR:OG1	2.09	0.69
1:B:338:ARG:NH2	1:B:358:PHE:O	2.30	0.65
1:D:350:LEU:HD22	1:D:352:TRP:CD1	2.32	0.64
1:F:144:ARG:NH2	1:F:158:SER:O	2.30	0.64
1:B:117:ARG:HG3	1:B:290:LEU:HD13	1.82	0.61
1:B:144:ARG:NH2	1:B:158:SER:O	2.31	0.61
1:C:117:ARG:HG3	1:C:290:LEU:HD13	1.83	0.61
1:B:301:GLN:OE1	1:D:33:THR:HG23	2.00	0.61
1:D:144:ARG:NH2	1:D:158:SER:O	2.35	0.60
1:F:373:ASP:OD1	1:F:375:GLY:N	2.31	0.60
1:F:146:ALA:O	1:F:147:THR:OG1	2.16	0.59
1:A:134:ARG:NH1	1:A:140:ARG:O	2.37	0.57
1:E:338:ARG:NH2	1:E:358:PHE:O	2.38	0.56
1:B:15:VAL:HG12	1:B:39:HIS:CE1	2.42	0.55
1:D:15:VAL:HG12	1:D:39:HIS:CE1	2.42	0.55
1:B:1:GLY:N	2:B:502:HOH:O	2.40	0.54
1:E:333:LEU:HB3	1:E:412:LEU:HD13	1.90	0.54
1:C:140:ARG:NH1	1:C:179:ASN:OD1	2.41	0.53
1:B:175:GLU:O	1:B:179:ASN:ND2	2.42	0.53
1:E:15:VAL:HG12	1:E:39:HIS:CE1	2.44	0.52
1:A:209:PRO:HB2	1:A:254:MET:HG2	1.92	0.51
1:C:15:VAL:HG12	1:C:39:HIS:CE1	2.46	0.51
1:F:112:SER:OG	1:F:255:GLN:OE1	2.14	0.50
1:B:209:PRO:HB2	1:B:254:MET:HG2	1.93	0.50
1:A:136:PHE:O	1:A:296:ARG:NH1	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:144:ARG:NH2	1:C:158:SER:O	2.44	0.49
1:F:335:GLN:OE1	1:F:338:ARG:NH1	2.44	0.49
1:E:154:ASP:OD1	1:E:154:ASP:N	2.46	0.48
1:F:188:ILE:HD11	1:F:226:GLU:HG2	1.97	0.47
1:F:115:LYS:NZ	1:F:284:GLU:OE2	2.48	0.47
1:D:147:THR:HA	1:D:160:TYR:O	2.15	0.47
1:D:394:ARG:NH1	1:D:404:ILE:O	2.47	0.47
1:A:190:GLY:O	1:A:194:VAL:HG23	2.15	0.47
1:C:386:ASP:OD1	1:C:387:VAL:N	2.47	0.47
1:A:333:LEU:HD22	1:A:421:VAL:HG21	1.98	0.46
1:E:211:GLY:HA2	1:E:219:VAL:HG12	1.96	0.46
1:E:192:ARG:HG2	1:E:230:LEU:HD11	1.98	0.46
1:B:136:PHE:O	1:B:296:ARG:NH1	2.49	0.45
1:F:126:THR:HG21	1:F:150:HIS:HB3	1.99	0.45
1:A:12:GLU:O	1:A:15:VAL:HG12	2.17	0.45
1:F:211:GLY:HA2	1:F:219:VAL:HG12	1.99	0.45
1:F:333:LEU:CD2	1:F:421:VAL:HG21	2.47	0.45
1:F:116:LEU:HD12	1:F:116:LEU:C	2.37	0.44
1:B:11:THR:O	1:B:15:VAL:HG13	2.17	0.44
1:E:63:PHE:CG	1:E:405:GLY:HA3	2.52	0.44
1:F:290:LEU:O	1:F:297:LYS:NZ	2.50	0.44
1:D:117:ARG:HG3	1:D:290:LEU:HD13	1.99	0.44
1:A:147:THR:HA	1:A:160:TYR:O	2.19	0.43
1:B:301:GLN:CD	1:D:33:THR:HG23	2.39	0.43
1:C:295:ASP:OD1	1:C:295:ASP:N	2.51	0.43
1:B:159:GLY:HA3	1:B:182:LEU:HD11	1.99	0.43
1:C:22:ARG:NH2	1:C:38:PRO:O	2.50	0.43
1:B:146:ALA:O	1:B:147:THR:OG1	2.22	0.43
1:C:134:ARG:NH1	1:C:140:ARG:O	2.45	0.43
1:C:190:GLY:O	1:C:194:VAL:HG23	2.20	0.42
1:E:147:THR:HA	1:E:160:TYR:O	2.20	0.42
1:E:333:LEU:HD22	1:E:421:VAL:HG21	2.01	0.42
1:D:116:LEU:HD12	1:D:116:LEU:C	2.39	0.42
1:C:34:ARG:NH1	2:C:501:HOH:O	2.47	0.42
1:E:116:LEU:C	1:E:116:LEU:HD12	2.39	0.42
1:E:379:ARG:NH1	1:E:381:GLU:OE1	2.52	0.42
1:D:362:HIS:ND1	1:D:409:SER:OG	2.38	0.41
1:C:285:ASP:N	1:C:285:ASP:OD1	2.53	0.41
1:B:98:LEU:HD12	1:B:308:PRO:HB3	2.03	0.41
1:A:333:LEU:HB3	1:A:412:LEU:HD13	2.02	0.41
1:F:394:ARG:NH2	1:F:404:ILE:O	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:96:HIS:O	1:C:99:GLU:HG2	2.22	0.40
1:E:285:ASP:N	1:E:285:ASP:OD1	2.53	0.40
1:F:404:ILE:HD12	1:F:408:GLY:HA2	2.03	0.40
1:F:136:PHE:O	1:F:296:ARG:NH1	2.54	0.40
1:A:30:THR:HA	1:C:117:ARG:HD3	2.02	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	440/464 (95%)	427 (97%)	12 (3%)	1 (0%)	47	53
1	B	438/464 (94%)	428 (98%)	9 (2%)	1 (0%)	47	53
1	C	437/464 (94%)	424 (97%)	13 (3%)	0	100	100
1	D	438/464 (94%)	422 (96%)	16 (4%)	0	100	100
1	E	433/464 (93%)	420 (97%)	13 (3%)	0	100	100
1	F	435/464 (94%)	419 (96%)	16 (4%)	0	100	100
All	All	2621/2784 (94%)	2540 (97%)	79 (3%)	2 (0%)	51	58

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	406	GLY
1	A	408	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	344/363 (95%)	338 (98%)	6 (2%)	60	68
1	B	342/363 (94%)	333 (97%)	9 (3%)	46	52
1	C	342/363 (94%)	336 (98%)	6 (2%)	59	66
1	D	342/363 (94%)	335 (98%)	7 (2%)	55	62
1	E	340/363 (94%)	332 (98%)	8 (2%)	49	55
1	F	339/363 (93%)	333 (98%)	6 (2%)	59	66
All	All	2049/2178 (94%)	2007 (98%)	42 (2%)	55	62

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	ASN
1	A	23	SER
1	A	301	GLN
1	A	333	LEU
1	A	373	ASP
1	A	428	PHE
1	B	15	VAL
1	B	19	GLN
1	B	301	GLN
1	B	325	ASP
1	B	333	LEU
1	B	350	LEU
1	B	373	ASP
1	B	407	ARG
1	B	428	PHE
1	C	2	SER
1	C	15	VAL
1	C	292	ARG
1	C	333	LEU
1	C	350	LEU
1	C	428	PHE
1	D	15	VAL
1	D	188	ILE
1	D	333	LEU
1	D	350	LEU
1	D	351	ASN

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Mol	Chain	Res	Type
1	D	388	LYS
1	D	428	PHE
1	E	15	VAL
1	E	95	SER
1	E	154	ASP
1	E	325	ASP
1	E	333	LEU
1	E	350	LEU
1	E	373	ASP
1	E	428	PHE
1	F	165	ASP
1	F	226	GLU
1	F	325	ASP
1	F	333	LEU
1	F	389	MET
1	F	428	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA

There are no RNA molecules in this entry.

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

6 non-standard protein/DNA/RNA residues are modelled in this entry.

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	$\#\|Z\| > 2$
1	LLP	E	269	1	23,24,25	2.69	6 (26%)	25,32,34	1.23	3 (12%)
1	LLP	C	269	1	23,24,25	2.68	6 (26%)	25,32,34	1.27	2 (8%)
1	LLP	B	269	1	23,24,25	2.65	6 (26%)	25,32,34	1.35	3 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	LLP	D	269	1	23,24,25	2.69	6 (26%)	25,32,34	1.24	3 (12%)
1	LLP	F	269	1	23,24,25	2.68	6 (26%)	25,32,34	1.15	2 (8%)
1	LLP	A	269	1	23,24,25	2.69	6 (26%)	25,32,34	1.31	3 (12%)

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
1	LLP	E	269	1	-	10/16/17/19	0/1/1/1
1	LLP	C	269	1	-	4/16/17/19	0/1/1/1
1	LLP	B	269	1	-	6/16/17/19	0/1/1/1
1	LLP	D	269	1	-	5/16/17/19	0/1/1/1
1	LLP	F	269	1	-	5/16/17/19	0/1/1/1
1	LLP	A	269	1	-	6/16/17/19	0/1/1/1

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	269	LLP	C4-C4'	8.71	1.63	1.46
1	E	269	LLP	C4-C4'	8.67	1.63	1.46
1	C	269	LLP	C4-C4'	8.60	1.63	1.46
1	D	269	LLP	C4-C4'	8.59	1.63	1.46
1	B	269	LLP	C4-C4'	8.53	1.62	1.46
1	F	269	LLP	C4-C4'	8.47	1.62	1.46
1	D	269	LLP	C4'-NZ	5.46	1.45	1.27
1	A	269	LLP	C4'-NZ	5.35	1.45	1.27
1	C	269	LLP	C4'-NZ	5.33	1.45	1.27
1	E	269	LLP	C4'-NZ	5.31	1.45	1.27
1	B	269	LLP	C4'-NZ	5.29	1.45	1.27
1	F	269	LLP	C4'-NZ	5.15	1.44	1.27
1	F	269	LLP	C4-C5	-3.95	1.37	1.42
1	B	269	LLP	C2'-C2	3.77	1.56	1.50
1	E	269	LLP	C4-C5	-3.69	1.37	1.42
1	A	269	LLP	C2'-C2	3.67	1.56	1.50
1	C	269	LLP	C2'-C2	3.62	1.56	1.50
1	A	269	LLP	C4-C5	-3.58	1.37	1.42
1	D	269	LLP	C2'-C2	3.57	1.56	1.50
1	E	269	LLP	C2'-C2	3.56	1.56	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	269	LLP	C4-C5	-3.56	1.37	1.42
1	C	269	LLP	C4-C5	-3.56	1.37	1.42
1	F	269	LLP	C2'-C2	3.52	1.56	1.50
1	D	269	LLP	C4-C5	-3.51	1.37	1.42
1	F	269	LLP	C6-N1	3.09	1.40	1.34
1	E	269	LLP	C6-N1	3.03	1.40	1.34
1	C	269	LLP	C6-N1	2.96	1.40	1.34
1	D	269	LLP	C6-N1	2.95	1.40	1.34
1	A	269	LLP	C6-N1	2.95	1.40	1.34
1	B	269	LLP	C6-N1	2.81	1.40	1.34
1	C	269	LLP	C5'-C5	2.15	1.56	1.50
1	E	269	LLP	C5'-C5	2.10	1.56	1.50
1	F	269	LLP	C5'-C5	2.09	1.56	1.50
1	D	269	LLP	C5'-C5	2.08	1.56	1.50
1	A	269	LLP	C5'-C5	2.05	1.56	1.50
1	B	269	LLP	C5'-C5	2.01	1.56	1.50

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	269	LLP	C4-C4'-NZ	-3.49	108.29	124.31
1	F	269	LLP	C4-C4'-NZ	-3.46	108.44	124.31
1	C	269	LLP	C4-C4'-NZ	-3.37	108.85	124.31
1	A	269	LLP	C4-C4'-NZ	-3.36	108.86	124.31
1	D	269	LLP	C4-C4'-NZ	-3.30	109.14	124.31
1	E	269	LLP	C4-C4'-NZ	-3.20	109.60	124.31
1	B	269	LLP	C4-C3-C2	2.70	121.86	120.19
1	A	269	LLP	C4-C3-C2	2.57	121.78	120.19
1	C	269	LLP	C4-C3-C2	2.42	121.69	120.19
1	A	269	LLP	OP4-C5'-C5	2.37	113.87	109.35
1	B	269	LLP	OP4-C5'-C5	2.25	113.64	109.35
1	E	269	LLP	OP4-C5'-C5	2.22	113.57	109.35
1	D	269	LLP	OP4-C5'-C5	2.19	113.52	109.35
1	D	269	LLP	C4-C3-C2	2.16	121.53	120.19
1	E	269	LLP	C4-C3-C2	2.11	121.49	120.19
1	F	269	LLP	C5-C6-N1	-2.10	120.32	123.82

There are no chirality outliers.

All (36) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	E	269	LLP	C4-C5-C5'-OP4

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Mol	Chain	Res	Type	Atoms
1	E	269	LLP	C6-C5-C5'-OP4
1	E	269	LLP	C5'-OP4-P-OP2
1	E	269	LLP	C5'-OP4-P-OP3
1	E	269	LLP	O-C-CA-CB
1	C	269	LLP	O-C-CA-CB
1	B	269	LLP	O-C-CA-CB
1	D	269	LLP	C4-C4'-NZ-CE
1	D	269	LLP	O-C-CA-CB
1	D	269	LLP	CG-CD-CE-NZ
1	F	269	LLP	O-C-CA-CB
1	A	269	LLP	O-C-CA-CB
1	A	269	LLP	CG-CD-CE-NZ
1	E	269	LLP	C4-C4'-NZ-CE
1	C	269	LLP	C4-C4'-NZ-CE
1	A	269	LLP	C4-C4'-NZ-CE
1	B	269	LLP	C4-C4'-NZ-CE
1	F	269	LLP	C4-C4'-NZ-CE
1	E	269	LLP	CG-CD-CE-NZ
1	C	269	LLP	CG-CD-CE-NZ
1	B	269	LLP	CG-CD-CE-NZ
1	F	269	LLP	C3-C4-C4'-NZ
1	E	269	LLP	C5'-OP4-P-OP1
1	E	269	LLP	CD-CE-NZ-C4'
1	B	269	LLP	C3-C4-C4'-NZ
1	D	269	LLP	C3-C4-C4'-NZ
1	E	269	LLP	C3-C4-C4'-NZ
1	A	269	LLP	C3-C4-C4'-NZ
1	F	269	LLP	CD-CE-NZ-C4'
1	D	269	LLP	CD-CE-NZ-C4'
1	A	269	LLP	CD-CE-NZ-C4'
1	B	269	LLP	C5'-OP4-P-OP2
1	A	269	LLP	C5'-OP4-P-OP2
1	B	269	LLP	CD-CE-NZ-C4'
1	C	269	LLP	C3-C4-C4'-NZ
1	F	269	LLP	C5-C4-C4'-NZ

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

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	442/464 (95%)	0.45	41 (9%) 8 8	34, 47, 73, 89	0
1	B	440/464 (94%)	0.25	22 (5%) 28 28	34, 49, 74, 100	0
1	C	439/464 (94%)	0.54	49 (11%) 5 4	34, 55, 86, 125	0
1	D	440/464 (94%)	0.47	39 (8%) 9 9	32, 52, 78, 108	0
1	E	437/464 (94%)	0.64	55 (12%) 3 2	44, 63, 95, 121	0
1	F	437/464 (94%)	1.00	86 (19%) 1 1	56, 80, 106, 124	0
All	All	2635/2784 (94%)	0.56	292 (11%) 5 4	32, 57, 94, 125	0

All (292) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	350	LEU	6.9
1	F	196	ALA	5.7
1	C	120	GLY	5.1
1	C	123	THR	4.9
1	F	352	TRP	4.8
1	A	121	SER	4.8
1	A	303	THR	4.7
1	C	121	SER	4.7
1	A	120	GLY	4.7
1	F	382	VAL	4.7
1	C	127	LEU	4.7
1	F	166	GLY	4.7
1	E	175	GLU	4.6
1	D	166	GLY	4.6
1	D	1	GLY	4.5
1	E	195	PHE	4.5
1	F	346	ALA	4.5
1	F	435	LEU	4.4
1	C	384	ARG	4.4

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Mol	Chain	Res	Type	RSRZ
1	A	302	GLY	4.3
1	F	171	GLY	4.3
1	F	163	HIS	4.3
1	A	119	THR	4.3
1	A	123	THR	4.3
1	C	119	THR	4.3
1	F	168	PRO	4.3
1	F	232	ARG	4.2
1	E	120	GLY	4.2
1	B	175	GLU	4.1
1	C	122	GLY	4.1
1	A	305	THR	4.1
1	E	164	PHE	4.1
1	C	125	THR	4.0
1	A	278	GLY	4.0
1	C	152	TRP	3.9
1	F	384	ARG	3.9
1	F	380	ALA	3.9
1	E	384	ARG	3.9
1	C	302	GLY	3.9
1	F	164	PHE	3.9
1	A	152	TRP	3.8
1	A	304	PHE	3.8
1	F	92	TYR	3.8
1	F	233	GLN	3.8
1	C	276	PRO	3.8
1	A	125	THR	3.7
1	F	347	ARG	3.7
1	A	126	THR	3.7
1	D	439	ASN	3.7
1	E	302	GLY	3.7
1	D	152	TRP	3.7
1	F	165	ASP	3.7
1	E	178	LYS	3.7
1	F	383	ALA	3.6
1	C	126	THR	3.6
1	F	125	THR	3.6
1	F	199	GLY	3.6
1	F	345	PHE	3.6
1	E	194	VAL	3.6
1	C	382	VAL	3.6
1	E	174	PRO	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	301	GLN	3.5
1	C	305	THR	3.5
1	E	140	ARG	3.5
1	F	302	GLY	3.5
1	A	127	LEU	3.5
1	F	344	LEU	3.5
1	F	155	PHE	3.4
1	E	385	PRO	3.4
1	E	171	GLY	3.4
1	E	199	GLY	3.4
1	A	124	GLU	3.4
1	B	302	GLY	3.4
1	A	268	ALA	3.4
1	C	266	CYS	3.4
1	C	151	GLY	3.4
1	C	275	LEU	3.4
1	F	121	SER	3.3
1	C	303	THR	3.3
1	F	167	GLN	3.3
1	E	16	PHE	3.3
1	A	122	GLY	3.3
1	F	158	SER	3.3
1	F	333	LEU	3.3
1	A	266	CYS	3.2
1	D	121	SER	3.2
1	E	230	LEU	3.2
1	C	277	GLY	3.2
1	F	202	ILE	3.2
1	D	305	THR	3.2
1	E	173	LEU	3.2
1	C	163	HIS	3.2
1	C	407	ARG	3.2
1	C	124	GLU	3.2
1	C	243	VAL	3.2
1	F	174	PRO	3.2
1	C	268	ALA	3.1
1	A	276	PRO	3.1
1	F	243	VAL	3.1
1	A	277	GLY	3.1
1	F	122	GLY	3.1
1	C	304	PHE	3.1
1	F	268	ALA	3.1

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Mol	Chain	Res	Type	RSRZ
1	E	121	SER	3.1
1	D	119	THR	3.1
1	F	323	GLU	3.0
1	A	129	ALA	3.0
1	F	175	GLU	3.0
1	D	167	GLN	3.0
1	E	301	GLN	3.0
1	F	432	LEU	3.0
1	F	437	ASP	3.0
1	A	118	PHE	3.0
1	C	194	VAL	3.0
1	F	438	GLU	3.0
1	F	385	PRO	3.0
1	B	163	HIS	3.0
1	D	5	ASN	3.0
1	E	270	ALA	3.0
1	E	54	VAL	3.0
1	F	348	LYS	3.0
1	E	383	ALA	2.9
1	F	386	ASP	2.9
1	A	128	LEU	2.9
1	F	195	PHE	2.9
1	E	234	TYR	2.9
1	D	123	THR	2.9
1	F	436	ALA	2.9
1	F	433	ASP	2.9
1	E	163	HIS	2.9
1	F	123	THR	2.8
1	F	278	GLY	2.8
1	F	366	GLY	2.8
1	F	343	HIS	2.8
1	D	120	GLY	2.8
1	F	194	VAL	2.8
1	C	129	ALA	2.8
1	D	125	THR	2.8
1	B	304	PHE	2.8
1	A	280	LEU	2.8
1	C	128	LEU	2.8
1	F	120	GLY	2.8
1	F	305	THR	2.8
1	D	276	PRO	2.8
1	D	140	ARG	2.8

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Mol	Chain	Res	Type	RSRZ
1	F	322	LEU	2.7
1	D	243	VAL	2.7
1	A	310	THR	2.7
1	D	3	ILE	2.7
1	E	278	GLY	2.7
1	E	197	GLN	2.7
1	A	16	PHE	2.7
1	F	178	LYS	2.7
1	F	388	LYS	2.7
1	C	167	GLN	2.7
1	E	200	SER	2.7
1	B	121	SER	2.7
1	F	276	PRO	2.7
1	E	134	ARG	2.7
1	E	196	ALA	2.7
1	C	301	GLN	2.7
1	D	277	GLY	2.7
1	A	165	ASP	2.7
1	F	127	LEU	2.7
1	D	279	ILE	2.6
1	E	122	GLY	2.6
1	B	174	PRO	2.6
1	F	365	PRO	2.6
1	A	279	ILE	2.6
1	F	244	ILE	2.6
1	C	278	GLY	2.6
1	D	151	GLY	2.6
1	D	2	SER	2.6
1	B	178	LYS	2.6
1	E	277	GLY	2.6
1	C	168	PRO	2.6
1	C	171	GLY	2.6
1	B	301	GLN	2.5
1	D	165	ASP	2.5
1	B	122	GLY	2.5
1	E	275	LEU	2.5
1	E	189	GLU	2.5
1	E	226	GLU	2.5
1	E	304	PHE	2.5
1	B	120	GLY	2.5
1	B	277	GLY	2.5
1	F	367	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	270	ALA	2.5
1	D	9	ARG	2.4
1	F	351	ASN	2.4
1	C	165	ASP	2.4
1	D	388	LYS	2.4
1	D	278	GLY	2.4
1	E	123	THR	2.4
1	E	188	ILE	2.4
1	D	440	LEU	2.4
1	F	157	ALA	2.4
1	F	389	MET	2.4
1	A	300	HIS	2.4
1	A	9	ARG	2.4
1	B	276	PRO	2.4
1	D	268	ALA	2.4
1	C	172	VAL	2.4
1	B	167	GLN	2.4
1	E	3	ILE	2.3
1	D	122	GLY	2.3
1	D	306	GLY	2.3
1	D	118	PHE	2.3
1	C	153	HIS	2.3
1	F	169	ALA	2.3
1	E	305	THR	2.3
1	F	119	THR	2.3
1	C	274	GLY	2.3
1	E	138	GLY	2.3
1	A	243	VAL	2.3
1	F	277	GLY	2.3
1	F	183	ILE	2.3
1	E	119	THR	2.3
1	C	166	GLY	2.3
1	E	306	GLY	2.3
1	D	304	PHE	2.3
1	D	175	GLU	2.3
1	E	201	ASP	2.3
1	C	30	THR	2.3
1	E	182	LEU	2.3
1	F	1	GLY	2.3
1	D	66	HIS	2.3
1	A	272	ALA	2.3
1	F	173	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	F	371	THR	2.2
1	F	66	HIS	2.2
1	E	170	PRO	2.2
1	E	181	LEU	2.2
1	A	270	ALA	2.2
1	B	303	THR	2.2
1	A	275	LEU	2.2
1	F	162	SER	2.2
1	C	383	ALA	2.2
1	E	9	ARG	2.2
1	F	141	MET	2.2
1	A	274	GLY	2.2
1	F	230	LEU	2.2
1	E	184	ARG	2.2
1	C	130	LEU	2.2
1	F	140	ARG	2.1
1	F	431	VAL	2.1
1	F	392	ALA	2.1
1	E	124	GLU	2.1
1	B	165	ASP	2.1
1	D	266	CYS	2.1
1	E	233	GLN	2.1
1	F	301	GLN	2.1
1	B	166	GLY	2.1
1	B	123	THR	2.1
1	E	118	PHE	2.1
1	F	428	PHE	2.1
1	F	279	ILE	2.1
1	A	267	LEU	2.1
1	E	158	SER	2.1
1	E	179	ASN	2.1
1	F	280	LEU	2.1
1	B	140	ARG	2.1
1	D	184	ARG	2.1
1	A	265	THR	2.1
1	F	201	ASP	2.1
1	B	152	TRP	2.1
1	C	90	VAL	2.1
1	F	407	ARG	2.1
1	C	66	HIS	2.1
1	C	300	HIS	2.1
1	E	191	MET	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	381	GLU	2.1
1	D	303	THR	2.1
1	F	77	ARG	2.1
1	C	65	GLY	2.1
1	B	197	GLN	2.1
1	D	300	HIS	2.1
1	E	224	LEU	2.1
1	E	300	HIS	2.1
1	A	102	TRP	2.1
1	C	149	TYR	2.1
1	B	305	THR	2.0
1	D	281	GLY	2.0
1	B	323	GLU	2.0
1	A	66	HIS	2.0
1	A	306	GLY	2.0
1	D	302	GLY	2.0
1	F	9	ARG	2.0
1	A	90	VAL	2.0
1	C	271	SER	2.0
1	D	30	THR	2.0
1	F	376	SER	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (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. 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	B-factors(Å^2)	Q<0.9
1	LLP	F	269	24/25	0.91	0.27	65,82,100,101	0
1	LLP	E	269	24/25	0.92	0.27	54,69,80,83	0
1	LLP	B	269	24/25	0.95	0.22	37,50,60,62	0
1	LLP	D	269	24/25	0.95	0.27	40,54,63,64	0
1	LLP	C	269	24/25	0.95	0.33	46,59,72,72	0
1	LLP	A	269	24/25	0.95	0.29	36,52,62,63	0

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.