Full wwPDB X-ray Structure Validation Report ⓘ

Apr 12, 2016 – 10:43 AM EDT

PDB ID	:	4QG5
Title	:	Crystal structure of phosphoglucomutase from Leishmania major at 3.5 angstrom resolution
Authors	:	Waugh, B.; Sen, U.; Banerjee, R.
Deposited on	:	2014-05-22
Resolution	:	3.50 Å(reported)

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

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

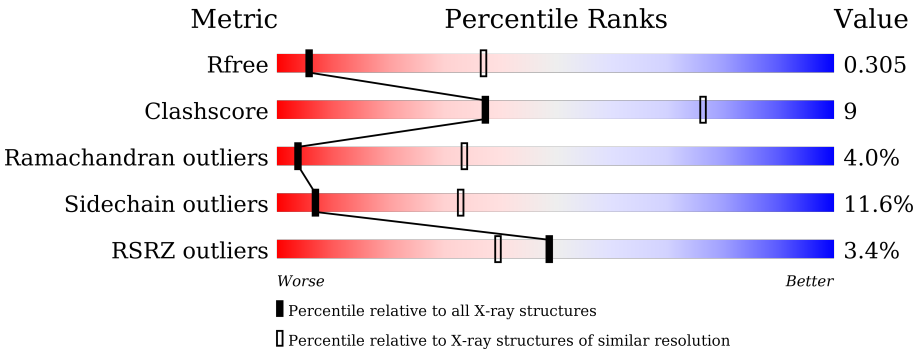
MolProbity	:	4.02b-467
Mogul	:	unknown
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20027107
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027107

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.50 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	1051 (3.60-3.40)
Clashscore	102246	1157 (3.60-3.40)
Ramachandran outliers	100387	1120 (3.60-3.40)
Sidechain outliers	100360	1121 (3.60-3.40)
RSRZ outliers	91569	1058 (3.60-3.40)

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	592	4% 67% 23% 5% • 5%
1	B	592	2% 68% 22% • • 6%
1	C	592	3% 69% 22% • 5%
1	D	592	3% 69% 21% • • 6%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 17136 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 Putative phosphoglucomutase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	565	Total	C	N	O	S	0	0	0
			4320	2733	738	832	17			
1	B	559	Total	C	N	O	S	0	0	0
			4264	2696	729	822	17			
1	C	561	Total	C	N	O	S	0	0	0
			4284	2709	732	826	17			
1	D	559	Total	C	N	O	S	0	0	0
			4264	2696	729	822	17			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	EXPRESSION TAG	UNP Q4QCF1
A	-1	SER	-	EXPRESSION TAG	UNP Q4QCF1
A	0	HIS	-	EXPRESSION TAG	UNP Q4QCF1
B	-2	GLY	-	EXPRESSION TAG	UNP Q4QCF1
B	-1	SER	-	EXPRESSION TAG	UNP Q4QCF1
B	0	HIS	-	EXPRESSION TAG	UNP Q4QCF1
C	-2	GLY	-	EXPRESSION TAG	UNP Q4QCF1
C	-1	SER	-	EXPRESSION TAG	UNP Q4QCF1
C	0	HIS	-	EXPRESSION TAG	UNP Q4QCF1
D	-2	GLY	-	EXPRESSION TAG	UNP Q4QCF1
D	-1	SER	-	EXPRESSION TAG	UNP Q4QCF1
D	0	HIS	-	EXPRESSION TAG	UNP Q4QCF1

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

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

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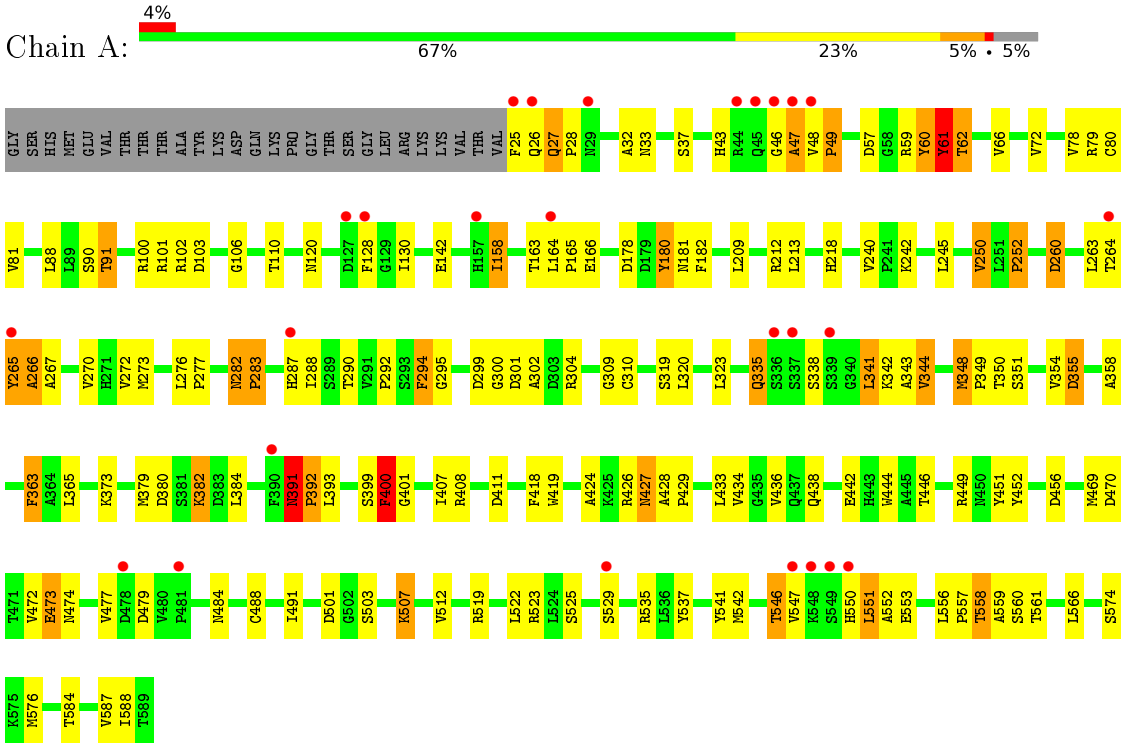
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	D	1	Total Mg 1 1	0	0
2	C	1	Total Mg 1 1	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

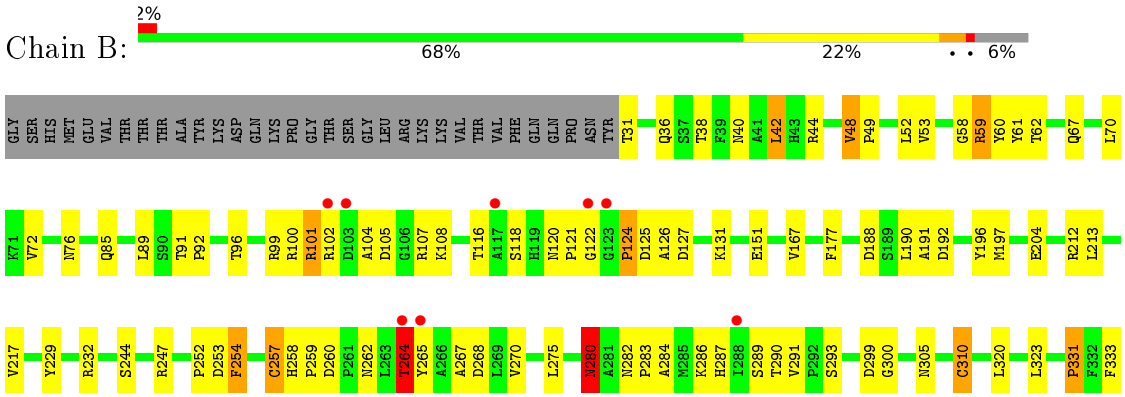
- Molecule 1: Putative phosphoglucomutase

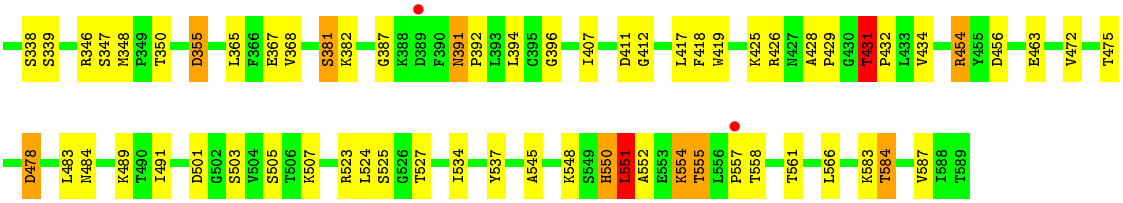
Chain A:

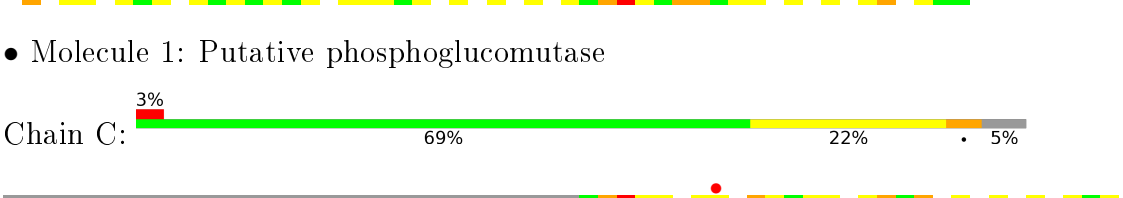


- Molecule 1: Putative phosphoglucomutase

Chain B:

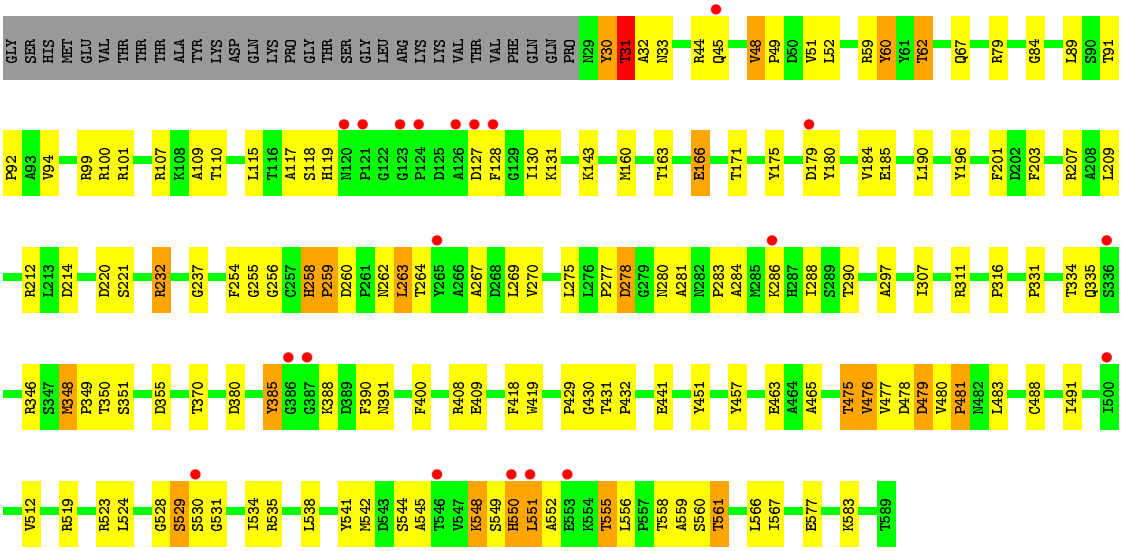






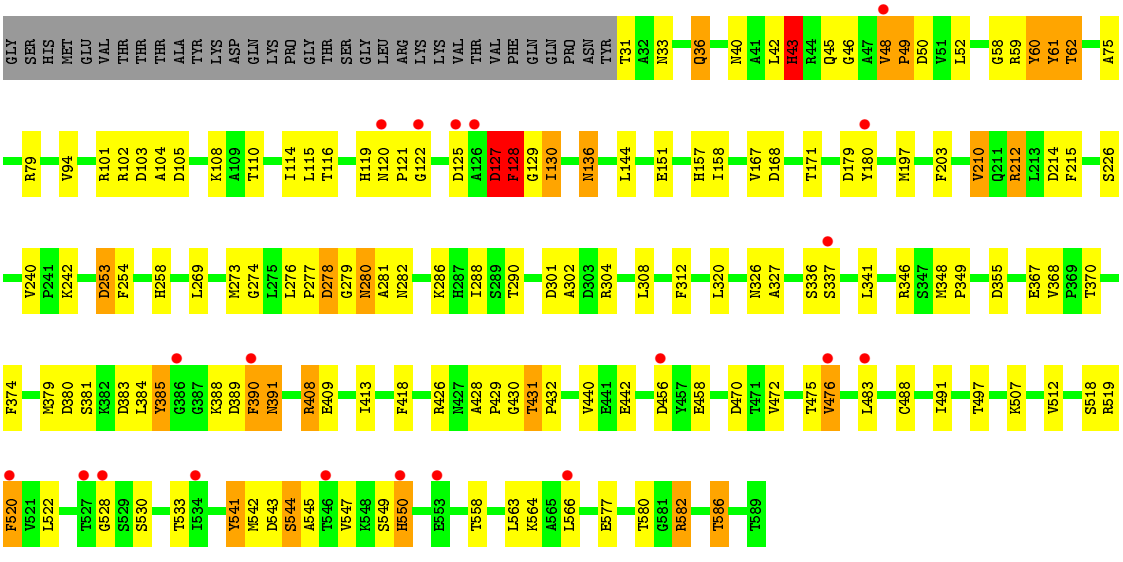
• Molecule 1: Putative phosphoglucomutase

Chain C:



• Molecule 1: Putative phosphoglucomutase

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	202.36Å 114.97Å 125.92Å 90.00° 110.03° 90.00°	Depositor
Resolution (Å)	38.17 – 3.50 39.65 – 3.50	Depositor EDS
% Data completeness (in resolution range)	86.3 (38.17-3.50) 79.5 (39.65-3.50)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.68 (at 3.48Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.238 , 0.315 0.235 , 0.305	Depositor DCC
R_{free} test set	1374 reflections (5.04%)	DCC
Wilson B-factor (Å^2)	66.8	Xtriage
Anisotropy	0.778	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 62.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.28$	Xtriage
Outliers	0 of 29657 reflections	Xtriage
F_o,F_c correlation	0.86	EDS
Total number of atoms	17136	wwPDB-VP
Average B, all atoms (Å^2)	76.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.32% 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: 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	0.33	0/4421	0.52	0/6016
1	B	0.31	0/4362	0.52	1/5935 (0.0%)
1	C	0.31	0/4383	0.52	1/5964 (0.0%)
1	D	0.32	0/4362	0.52	0/5935
All	All	0.32	0/17528	0.52	2/23850 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	550	HIS	C-N-CA	5.82	136.26	121.70
1	C	475	THR	C-N-CA	5.15	134.57	121.70

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	4320	0	4203	95	0
1	B	4264	0	4157	79	0
1	C	4284	0	4171	65	0
1	D	4264	0	4157	82	0
2	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
All	All	17136	0	16688	313	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 9.

All (313) 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:264:THR:O	1:A:266:ALA:N	2.12	0.82
1:B:31:THR:N	1:D:60:TYR:HH	1.82	0.77
1:A:48:VAL:O	1:A:79:ARG:NE	2.17	0.76
1:B:264:THR:OG1	1:B:265:TYR:N	2.18	0.75
1:C:346:ARG:NH1	1:C:350:THR:O	2.19	0.75
1:A:180:TYR:O	1:A:182:PHE:N	2.21	0.74
1:A:380:ASP:OD1	1:A:408:ARG:NH1	2.21	0.74
1:B:124:PRO:O	1:D:31:THR:N	2.23	0.72
1:C:441:GLU:OE1	1:C:550:HIS:ND1	2.22	0.72
1:C:475:THR:HA	1:C:476:VAL:HB	1.70	0.71
1:B:287:HIS:O	1:B:287:HIS:ND1	2.23	0.71
1:B:454:ARG:NH1	1:B:456:ASP:OD2	2.24	0.71
1:C:529:SER:O	1:C:531:GLY:N	2.24	0.70
1:D:127:ASP:O	1:D:129:GLY:N	2.26	0.68
1:D:380:ASP:OD1	1:D:408:ARG:NH1	2.27	0.68
1:A:391:ASN:O	1:A:393:LEU:N	2.26	0.68
1:D:101:ARG:HB3	1:D:102:ARG:HA	1.76	0.68
1:A:309:GLY:HA3	1:A:436:VAL:HG11	1.74	0.68
1:B:270:VAL:HG13	1:B:275:LEU:HB2	1.77	0.67
1:B:331:PRO:O	1:B:333:PHE:N	2.27	0.67
1:B:550:HIS:HB2	1:B:551:LEU:HB3	1.76	0.67
1:B:554:LYS:O	1:B:555:THR:OG1	2.13	0.66
1:D:274:GLY:O	1:D:282:ASN:ND2	2.29	0.65
1:C:380:ASP:OD1	1:C:408:ARG:NH1	2.29	0.65
1:B:99:ARG:O	1:B:108:LYS:NZ	2.28	0.65
1:C:283:PRO:N	1:C:284:ALA:HA	2.11	0.65
1:C:476:VAL:O	1:C:478:ASP:N	2.29	0.65
1:A:276:LEU:HD21	1:A:283:PRO:HG3	1.79	0.65
1:D:389:ASP:O	1:D:391:ASN:N	2.30	0.64
1:D:426:ARG:NH1	1:D:442:GLU:OE1	2.30	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:550:HIS:N	1:B:551:LEU:HB3	2.12	0.64
1:B:247:ARG:NH2	1:B:268:ASP:OD2	2.29	0.64
1:D:101:ARG:CB	1:D:102:ARG:HA	2.28	0.63
1:A:60:TYR:HB2	1:A:252:PRO:HB3	1.80	0.62
1:B:188:ASP:OD1	1:B:191:ALA:N	2.32	0.62
1:B:280:ASN:N	1:B:280:ASN:OD1	2.32	0.62
1:C:220:ASP:OD1	1:C:221:SER:N	2.33	0.61
1:A:62:THR:O	1:A:66:VAL:N	2.35	0.60
1:B:348:MET:N	1:B:368:VAL:O	2.35	0.60
1:C:475:THR:HA	1:C:476:VAL:CB	2.32	0.59
1:B:260:ASP:O	1:B:262:ASN:ND2	2.36	0.59
1:B:67:GLN:NE2	1:B:167:VAL:O	2.36	0.58
1:A:163:THR:H	1:A:164:LEU:HA	1.68	0.58
1:A:343:ALA:HB3	1:A:393:LEU:HA	1.85	0.58
1:B:217:VAL:O	1:B:244:SER:OG	2.21	0.58
1:B:550:HIS:CA	1:B:551:LEU:HB3	2.34	0.58
1:A:546:THR:HB	1:A:547:VAL:HG12	1.86	0.57
1:B:346:ARG:NH1	1:B:350:THR:O	2.38	0.57
1:A:283:PRO:HB2	1:D:75:ALA:HA	1.86	0.57
1:B:59:ARG:HD2	1:B:60:TYR:N	2.19	0.57
1:B:411:ASP:OD1	1:B:412:GLY:N	2.38	0.57
1:D:116:THR:HG21	1:D:301:ASP:HB3	1.87	0.57
1:C:101:ARG:NH2	1:C:185:GLU:OE2	2.37	0.56
1:D:456:ASP:O	1:D:586:THR:OG1	2.22	0.56
1:B:501:ASP:OD2	1:B:503:SER:N	2.38	0.56
1:B:126:ALA:HB2	1:D:125:ASP:HB2	1.85	0.56
1:A:355:ASP:OD1	1:A:355:ASP:N	2.39	0.56
1:A:48:VAL:N	1:A:49:PRO:HD3	2.21	0.56
1:C:89:LEU:HD22	1:C:94:VAL:HG22	1.88	0.56
1:A:163:THR:N	1:A:164:LEU:HA	2.22	0.55
1:A:319:SER:HG	1:A:419:TRP:HE1	1.53	0.55
1:A:265:TYR:C	1:A:267:ALA:H	2.10	0.54
1:B:267:ALA:HA	1:B:270:VAL:HB	1.89	0.54
1:B:59:ARG:HH12	1:B:121:PRO:CA	2.21	0.54
1:D:168:ASP:OD1	1:D:171:THR:N	2.40	0.54
1:A:163:THR:HG22	1:A:165:PRO:HD3	1.88	0.54
1:D:429:PRO:N	1:D:430:GLY:HA3	2.22	0.54
1:C:117:ALA:O	1:C:119:HIS:N	2.41	0.53
1:A:350:THR:O	1:A:519:ARG:NH2	2.42	0.53
1:B:36:GLN:NE2	1:B:40:ASN:OD1	2.42	0.53
1:C:451:TYR:HD1	1:C:559:ALA:HB2	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:512:VAL:HB	1:D:520:PHE:HB3	1.91	0.53
1:A:32:ALA:HB1	1:A:72:VAL:HG21	1.90	0.53
1:C:429:PRO:N	1:C:430:GLY:HA3	2.24	0.53
1:A:309:GLY:HA3	1:A:436:VAL:CG1	2.39	0.53
1:B:59:ARG:HH12	1:B:121:PRO:HA	1.74	0.53
1:C:31:THR:O	1:C:33:ASN:N	2.42	0.53
1:D:543:ASP:O	1:D:545:ALA:N	2.42	0.53
1:B:299:ASP:OD2	1:B:300:GLY:N	2.40	0.52
1:C:269:LEU:HD22	1:C:297:ALA:HB2	1.91	0.52
1:D:383:ASP:O	1:D:385:TYR:N	2.42	0.52
1:B:124:PRO:HD3	1:B:254:PHE:HB3	1.92	0.52
1:C:264:THR:HG21	1:C:277:PRO:HA	1.92	0.52
1:B:550:HIS:CB	1:B:551:LEU:HB3	2.39	0.52
1:C:99:ARG:HG3	1:C:100:ARG:HG2	1.92	0.52
1:D:62:THR:HG23	1:D:115:LEU:HD22	1.91	0.51
1:C:538:LEU:HD13	1:C:567:ILE:HG12	1.92	0.51
1:A:379:MET:CG	1:A:393:LEU:HD23	2.41	0.51
1:D:346:ARG:NH2	1:D:367:GLU:OE1	2.43	0.51
1:D:327:ALA:HB3	1:D:341:LEU:HD22	1.92	0.51
1:A:342:LYS:O	1:A:343:ALA:HB2	2.11	0.51
1:C:560:SER:HB3	1:C:561:THR:HA	1.92	0.50
1:A:304:ARG:HA	1:A:401:GLY:HA2	1.93	0.50
1:B:116:THR:HG22	1:B:118:SER:H	1.76	0.50
1:D:46:GLY:N	1:D:50:ASP:OD2	2.38	0.50
1:C:475:THR:N	1:C:476:VAL:HG23	2.25	0.50
1:D:210:VAL:HG11	1:D:240:VAL:HG22	1.94	0.50
1:B:289:SER:HB3	1:B:290:THR:HA	1.94	0.50
1:B:523:ARG:NH1	1:B:537:TYR:OH	2.44	0.50
1:B:524:LEU:HD22	1:B:534:ILE:HA	1.93	0.50
1:B:91:THR:HB	1:B:92:PRO:HD3	1.94	0.50
1:D:212:ARG:NH1	1:D:214:ASP:OD1	2.45	0.50
1:D:549:SER:HA	1:D:550:HIS:C	2.32	0.49
1:B:120:ASN:ND2	1:B:120:ASN:O	2.42	0.49
1:A:424:ALA:O	1:A:426:ARG:N	2.45	0.49
1:A:472:VAL:HG21	1:A:522:LEU:CD1	2.41	0.49
1:D:226:SER:HB3	1:D:302:ALA:HB2	1.94	0.49
1:B:391:ASN:OD1	1:B:391:ASN:N	2.46	0.49
1:C:277:PRO:N	1:C:278:ASP:HA	2.28	0.49
1:D:101:ARG:HB3	1:D:102:ARG:CA	2.42	0.49
1:D:40:ASN:HB2	1:D:151:GLU:HG2	1.95	0.49
1:A:373:LYS:NZ	1:A:501:ASP:OD2	2.38	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:136:ASN:OD1	1:D:136:ASN:N	2.45	0.49
1:A:349:PRO:HB3	1:A:537:TYR:CE2	2.48	0.48
1:B:347:SER:OG	1:B:350:THR:OG1	2.30	0.48
1:D:101:ARG:HB3	1:D:102:ARG:CG	2.43	0.48
1:D:59:ARG:NH1	1:D:253:ASP:HB3	2.28	0.48
1:D:367:GLU:OE1	1:D:519:ARG:NH1	2.46	0.48
1:A:379:MET:HG3	1:A:393:LEU:HD23	1.95	0.48
1:D:276:LEU:HB3	1:D:277:PRO:HD2	1.96	0.48
1:D:60:TYR:HB2	1:D:122:GLY:HA3	1.95	0.48
1:A:428:ALA:N	1:A:429:PRO:CD	2.77	0.48
1:A:60:TYR:HB2	1:A:252:PRO:CB	2.43	0.48
1:A:282:ASN:ND2	1:D:180:TYR:OH	2.46	0.48
1:C:99:ARG:NH1	1:C:408:ARG:HG2	2.28	0.48
1:D:326:ASN:HD21	1:D:426:ARG:HH21	1.61	0.48
1:D:476:VAL:HG22	1:D:491:ILE:CG2	2.44	0.48
1:A:90:SER:HB2	1:A:302:ALA:HB3	1.96	0.47
1:A:288:ILE:HG22	1:A:290:THR:H	1.79	0.47
1:D:580:THR:HG23	1:D:582:ARG:H	1.79	0.47
1:D:120:ASN:HB2	1:D:121:PRO:HD2	1.95	0.47
1:D:341:LEU:HD23	1:D:341:LEU:N	2.30	0.47
1:C:264:THR:HB	1:C:267:ALA:HA	1.96	0.47
1:D:541:TYR:HE2	1:D:543:ASP:HA	1.79	0.47
1:A:267:ALA:HA	1:A:270:VAL:HB	1.96	0.47
1:A:391:ASN:N	1:A:392:PRO:CD	2.77	0.47
1:C:480:VAL:HG13	1:C:481:PRO:HD2	1.96	0.47
1:C:488:CYS:HB2	1:C:491:ILE:HD11	1.97	0.47
1:A:477:VAL:HA	1:A:491:ILE:CD1	2.45	0.47
1:C:190:LEU:HD21	1:C:232:ARG:HG2	1.96	0.47
1:D:543:ASP:OD1	1:D:544:SER:N	2.42	0.47
1:B:96:THR:O	1:B:100:ARG:N	2.46	0.47
1:C:51:VAL:HB	1:C:109:ALA:HA	1.96	0.47
1:D:94:VAL:HG11	1:D:114:ILE:HG12	1.97	0.47
1:B:425:LYS:HA	1:B:426:ARG:C	2.36	0.47
1:A:537:TYR:N	1:A:537:TYR:HD1	2.13	0.46
1:A:400:PHE:CD2	1:A:400:PHE:N	2.82	0.46
1:A:546:THR:HB	1:A:547:VAL:HA	1.97	0.46
1:A:551:LEU:O	1:A:553:GLU:N	2.49	0.46
1:A:451:TYR:CE1	1:A:559:ALA:HA	2.50	0.46
1:A:456:ASP:HB2	1:A:587:VAL:HB	1.98	0.46
1:D:103:ASP:OD1	1:D:104:ALA:N	2.49	0.46
1:D:103:ASP:OD1	1:D:105:ASP:N	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:33:ASN:O	1:A:37:SER:OG	2.21	0.46
1:B:104:ALA:O	1:B:105:ASP:HB3	2.15	0.46
1:C:44:ARG:NH1	1:C:45:GLN:OE1	2.48	0.46
1:D:472:VAL:O	1:D:476:VAL:HB	2.16	0.46
1:B:524:LEU:CD2	1:B:534:ILE:HA	2.46	0.46
1:B:550:HIS:HB2	1:B:551:LEU:CB	2.46	0.46
1:C:280:ASN:OD1	1:C:281:ALA:N	2.47	0.46
1:B:188:ASP:OD2	1:B:232:ARG:NH2	2.48	0.46
1:B:212:ARG:HG2	1:B:213:LEU:N	2.31	0.46
1:B:60:TYR:HA	1:B:61:TYR:HA	1.73	0.46
1:B:320:LEU:HD13	1:B:396:GLY:HA3	1.97	0.46
1:D:45:GLN:N	1:D:46:GLY:HA2	2.30	0.46
1:A:537:TYR:N	1:A:537:TYR:CD1	2.84	0.45
1:A:546:THR:CB	1:A:547:VAL:HA	2.45	0.45
1:D:128:PHE:N	1:D:128:PHE:CD2	2.83	0.45
1:A:78:VAL:HG23	1:A:182:PHE:HE1	1.81	0.45
1:B:472:VAL:HA	1:B:475:THR:HG22	1.97	0.45
1:A:91:THR:OG1	1:A:301:ASP:O	2.33	0.45
1:A:470:ASP:O	1:A:474:ASN:N	2.49	0.45
1:C:348:MET:HB3	1:C:349:PRO:HD3	1.99	0.45
1:B:121:PRO:HG2	1:B:259:PRO:HG2	1.99	0.45
1:B:552:ALA:HB3	1:B:557:PRO:CD	2.45	0.45
1:C:552:ALA:HB3	1:C:555:THR:HA	1.99	0.45
1:C:270:VAL:HG13	1:C:275:LEU:HB2	1.99	0.45
1:D:212:ARG:CD	1:D:215:PHE:HB2	2.47	0.45
1:A:344:VAL:HG13	1:A:365:LEU:HA	1.99	0.45
1:B:40:ASN:HB2	1:B:151:GLU:HG2	1.99	0.45
1:A:428:ALA:CB	1:A:433:LEU:HB2	2.47	0.45
1:A:469:MET:CE	1:A:522:LEU:HB3	2.47	0.45
1:D:476:VAL:O	1:D:491:ILE:HD13	2.17	0.45
1:D:62:THR:O	1:D:62:THR:HG22	2.17	0.45
1:A:449:ARG:HD3	1:A:451:TYR:HE2	1.82	0.45
1:A:491:ILE:HG22	1:A:512:VAL:HA	1.97	0.45
1:D:278:ASP:O	1:D:280:ASN:N	2.50	0.45
1:A:473:GLU:C	1:A:477:VAL:HG23	2.37	0.44
1:A:407:ILE:HD11	1:A:411:ASP:HB2	1.99	0.44
1:B:42:LEU:C	1:B:42:LEU:HD23	2.37	0.44
1:C:212:ARG:HG2	1:C:214:ASP:H	1.83	0.44
1:B:323:LEU:HD21	1:B:419:TRP:CD1	2.53	0.44
1:A:59:ARG:HB3	1:A:252:PRO:HB3	2.00	0.44
1:B:289:SER:CB	1:B:290:THR:HA	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:101:ARG:CG	1:D:102:ARG:HA	2.48	0.44
1:A:260:ASP:N	1:A:260:ASP:OD2	2.50	0.44
1:A:434:VAL:HG13	1:A:438:GLN:CB	2.47	0.44
1:B:100:ARG:HG2	1:B:101:ARG:H	1.82	0.44
1:B:338:SER:HA	1:B:339:SER:HA	1.78	0.44
1:B:48:VAL:N	1:B:49:PRO:CD	2.81	0.44
1:C:463:GLU:OE2	1:C:463:GLU:N	2.44	0.44
1:A:294:PHE:HD1	1:A:295:GLY:N	2.15	0.44
1:B:428:ALA:N	1:B:429:PRO:CD	2.80	0.44
1:B:431:THR:H	1:B:432:PRO:HD2	1.82	0.44
1:C:541:TYR:HD2	1:C:542:MET:N	2.16	0.44
1:A:218:HIS:CD2	1:A:272:VAL:HG11	2.53	0.44
1:C:62:THR:HG23	1:C:115:LEU:HD13	2.00	0.44
1:B:456:ASP:HB2	1:B:587:VAL:HB	2.00	0.44
1:C:201:PHE:HA	1:C:331:PRO:HD2	1.99	0.44
1:C:465:ALA:HB1	1:C:524:LEU:HD11	1.99	0.44
1:C:451:TYR:CD1	1:C:559:ALA:HB2	2.51	0.44
1:D:368:VAL:HG11	1:D:374:PHE:HB2	1.99	0.44
1:B:391:ASN:HB2	1:B:392:PRO:HA	2.01	0.43
1:C:91:THR:HB	1:C:92:PRO:HD3	2.00	0.43
1:D:125:ASP:HB3	1:D:128:PHE:HB3	2.01	0.43
1:B:212:ARG:HG2	1:B:213:LEU:H	1.84	0.43
1:B:293:SER:HA	1:B:310:CYS:HB2	1.99	0.43
1:C:258:HIS:HA	1:C:259:PRO:HD3	1.94	0.43
1:A:382:LYS:HD3	1:A:382:LYS:H	1.83	0.43
1:B:167:VAL:HG12	1:B:177:PHE:HZ	1.83	0.43
1:B:475:THR:HA	1:B:478:ASP:HB3	1.99	0.43
1:D:341:LEU:HD23	1:D:341:LEU:H	1.83	0.43
1:A:541:TYR:CD2	1:A:542:MET:N	2.86	0.43
1:A:282:ASN:OD1	1:A:282:ASN:N	2.50	0.43
1:D:312:PHE:CZ	1:D:440:VAL:HG21	2.54	0.43
1:D:59:ARG:NH1	1:D:121:PRO:HG3	2.34	0.43
1:A:472:VAL:CG2	1:A:574:SER:HB3	2.48	0.43
1:B:382:LYS:HB2	1:B:387:GLY:HA2	2.01	0.43
1:D:476:VAL:HG13	1:D:491:ILE:HG21	2.00	0.43
1:C:175:TYR:N	1:C:184:VAL:O	2.47	0.43
1:D:488:CYS:SG	1:D:491:ILE:HD11	2.59	0.43
1:A:358:ALA:HA	1:A:363:PHE:CE1	2.54	0.43
1:A:473:GLU:O	1:A:477:VAL:HG23	2.18	0.43
1:A:444:TRP:CD2	1:A:449:ARG:HD2	2.54	0.42
1:B:122:GLY:O	1:B:254:PHE:HA	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:550:HIS:O	1:C:552:ALA:N	2.52	0.42
1:A:277:PRO:HG2	1:D:42:LEU:HD21	2.01	0.42
1:B:275:LEU:HD23	1:B:283:PRO:HA	1.99	0.42
1:C:549:SER:O	1:C:552:ALA:HB2	2.19	0.42
1:D:476:VAL:HG22	1:D:491:ILE:HG21	2.02	0.42
1:B:72:VAL:O	1:B:76:ASN:ND2	2.52	0.42
1:C:207:ARG:NH2	1:C:237:GLY:O	2.52	0.42
1:B:346:ARG:NH2	1:B:367:GLU:OE2	2.53	0.42
1:A:27:GLN:HB3	1:A:28:PRO:HD2	2.02	0.42
1:A:88:LEU:HD11	1:A:250:VAL:HG21	2.02	0.42
1:C:545:ALA:HB1	1:C:556:LEU:HD21	2.01	0.42
1:C:551:LEU:H	1:C:551:LEU:HD12	1.84	0.42
1:B:59:ARG:O	1:B:62:THR:OG1	2.20	0.42
1:D:59:ARG:O	1:D:61:TYR:N	2.52	0.42
1:B:52:LEU:HD23	1:B:53:VAL:N	2.35	0.42
1:A:128:PHE:CZ	1:A:130:ILE:HB	2.55	0.42
1:A:304:ARG:HA	1:A:401:GLY:CA	2.50	0.42
1:A:351:SER:HB2	1:A:452:TYR:CD1	2.55	0.42
1:C:457:TYR:HB2	1:C:534:ILE:HB	2.02	0.42
1:C:84:GLY:HA3	1:C:89:LEU:HD12	2.01	0.42
1:C:355:ASP:OD2	1:C:355:ASP:N	2.52	0.41
1:C:475:THR:CA	1:C:476:VAL:HG23	2.50	0.41
1:D:269:LEU:HG	1:D:308:LEU:HD12	2.01	0.41
1:A:80:CYS:SG	1:A:81:VAL:N	2.94	0.41
1:C:263:LEU:HA	1:C:264:THR:HA	1.82	0.41
1:D:355:ASP:N	1:D:355:ASP:OD2	2.53	0.41
1:D:476:VAL:HG13	1:D:491:ILE:CG2	2.50	0.41
1:A:342:LYS:H	1:A:392:PRO:HG2	1.84	0.41
1:A:309:GLY:CA	1:A:436:VAL:HG11	2.47	0.41
1:B:381:SER:HA	1:B:382:LYS:HA	1.89	0.41
1:B:355:ASP:OD1	1:B:355:ASP:N	2.53	0.41
1:B:320:LEU:HD12	1:B:394:LEU:HD21	2.02	0.41
1:C:316:PRO:HG3	1:C:400:PHE:CD1	2.56	0.41
1:C:48:VAL:CB	1:C:49:PRO:HA	2.51	0.41
1:D:130:ILE:O	1:D:130:ILE:HG23	2.20	0.41
1:D:541:TYR:HD2	1:D:542:MET:N	2.18	0.41
1:A:399:SER:O	1:A:400:PHE:O	2.38	0.41
1:A:551:LEU:HG	1:A:556:LEU:HD21	2.03	0.41
1:A:348:MET:N	1:A:349:PRO:CD	2.83	0.41
1:C:262:ASN:O	1:C:264:THR:HA	2.21	0.41
1:A:164:LEU:HD12	1:A:165:PRO:HD2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:59:ARG:HD2	1:B:60:TYR:O	2.20	0.41
1:C:491:ILE:HG13	1:C:512:VAL:HA	2.03	0.41
1:D:381:SER:HB2	1:D:390:PHE:HA	2.02	0.41
1:D:379:MET:HB3	1:D:408:ARG:HH21	1.85	0.41
1:D:45:GLN:N	1:D:46:GLY:CA	2.84	0.41
1:A:61:TYR:HD1	1:A:62:THR:N	2.19	0.41
1:B:190:LEU:HD23	1:B:229:TYR:CE2	2.55	0.41
1:D:312:PHE:CE2	1:D:440:VAL:HG21	2.55	0.41
1:A:273:MET:SD	1:A:292:PRO:HG2	2.60	0.41
1:C:171:THR:OG1	1:C:175:TYR:OH	2.35	0.41
1:C:370:THR:OG1	1:C:523:ARG:NH1	2.44	0.41
1:B:551:LEU:HD12	1:B:551:LEU:O	2.20	0.41
1:D:408:ARG:N	1:D:408:ARG:HD2	2.36	0.41
1:A:158:ILE:H	1:A:158:ILE:HD13	1.86	0.41
1:A:277:PRO:HB2	1:D:42:LEU:HD13	2.02	0.41
1:A:320:LEU:HD13	1:A:354:VAL:HG21	2.03	0.41
1:A:438:GLN:O	1:A:442:GLU:N	2.37	0.41
1:C:577:GLU:OE1	1:C:583:LYS:NZ	2.32	0.41
1:D:472:VAL:HA	1:D:475:THR:HG22	2.03	0.41
1:A:299:ASP:OD2	1:A:300:GLY:N	2.52	0.40
1:A:501:ASP:OD1	1:A:503:SER:N	2.49	0.40
1:A:588:ILE:HD12	1:D:43:HIS:HA	2.03	0.40
1:C:480:VAL:CG1	1:C:481:PRO:HD2	2.51	0.40
1:C:348:MET:HE1	1:C:519:ARG:NH1	2.37	0.40
1:D:348:MET:HB3	1:D:349:PRO:HD3	2.04	0.40
1:D:48:VAL:HB	1:D:49:PRO:HD3	2.04	0.40
1:D:428:ALA:HB1	1:D:431:THR:N	2.36	0.40
1:A:180:TYR:N	1:A:180:TYR:CD1	2.89	0.40
1:A:46:GLY:O	1:A:47:ALA:HB3	2.21	0.40
1:A:507:LYS:NZ	1:A:507:LYS:O	2.39	0.40
1:D:36:GLN:HG3	1:D:158:ILE:HA	2.03	0.40
1:D:458:GLU:HA	1:D:533:THR:HG23	2.02	0.40
1:C:30:TYR:CE2	1:C:128:PHE:HB3	2.56	0.40
1:C:48:VAL:HG11	1:C:79:ARG:NE	2.36	0.40
1:A:434:VAL:HG13	1:A:438:GLN:HB2	2.04	0.40
1:C:307:ILE:HD13	1:C:419:TRP:CD1	2.57	0.40
1:D:119:HIS:HA	1:D:120:ASN:HA	1.85	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	563/592 (95%)	454 (81%)	84 (15%)	25 (4%)	3	30
1	B	557/592 (94%)	478 (86%)	62 (11%)	17 (3%)	5	41
1	C	559/592 (94%)	467 (84%)	67 (12%)	25 (4%)	3	30
1	D	557/592 (94%)	464 (83%)	70 (13%)	23 (4%)	3	33
All	All	2236/2368 (94%)	1863 (83%)	283 (13%)	90 (4%)	4	33

All (90) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	61	TYR
1	A	181	ASN
1	A	265	TYR
1	A	283	PRO
1	A	400	PHE
1	A	560	SER
1	B	253	ASP
1	B	280	ASN
1	B	381	SER
1	B	545	ALA
1	C	258	HIS
1	C	286	LYS
1	C	476	VAL
1	C	477	VAL
1	C	530	SER
1	C	548	LYS
1	D	43	HIS
1	D	48	VAL
1	D	62	THR
1	D	127	ASP
1	D	128	PHE
1	A	47	ALA

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Mol	Chain	Res	Type
1	A	49	PRO
1	A	344	VAL
1	A	473	GLU
1	A	479	ASP
1	A	552	ALA
1	A	558	THR
1	B	127	ASP
1	B	310	CYS
1	B	551	LEU
1	C	31	THR
1	C	127	ASP
1	C	255	GLY
1	C	259	PRO
1	C	481	PRO
1	C	529	SER
1	D	49	PRO
1	D	130	ILE
1	D	279	GLY
1	D	336	SER
1	D	337	SER
1	D	384	LEU
1	D	390	PHE
1	D	432	PRO
1	D	530	SER
1	D	544	SER
1	A	310	CYS
1	A	341	LEU
1	A	550	HIS
1	B	257	CYS
1	B	284	ALA
1	B	331	PRO
1	B	555	THR
1	C	60	TYR
1	C	118	SER
1	C	166	GLU
1	C	544	SER
1	C	551	LEU
1	D	281	ALA
1	A	62	THR
1	A	252	PRO
1	A	266	ALA
1	A	335	GLN

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Mol	Chain	Res	Type
1	A	427	ASN
1	B	584	THR
1	C	256	GLY
1	C	385	TYR
1	C	555	THR
1	D	60	TYR
1	D	254	PHE
1	D	528	GLY
1	A	391	ASN
1	B	58	GLY
1	B	252	PRO
1	B	264	THR
1	B	431	THR
1	C	32	ALA
1	C	107	ARG
1	C	479	ASP
1	D	288	ILE
1	A	392	PRO
1	B	124	PRO
1	C	432	PRO
1	D	391	ASN
1	A	557	PRO
1	D	58	GLY
1	D	210	VAL
1	A	106	GLY
1	C	528	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	465/488 (95%)	406 (87%)	59 (13%)	5 28
1	B	459/488 (94%)	406 (88%)	53 (12%)	7 33
1	C	461/488 (94%)	414 (90%)	47 (10%)	9 40
1	D	459/488 (94%)	405 (88%)	54 (12%)	6 31

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1844/1952 (94%)	1631 (88%)	213 (12%)	7 33

All (213) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	PHE
1	A	26	GLN
1	A	27	GLN
1	A	43	HIS
1	A	57	ASP
1	A	60	TYR
1	A	61	TYR
1	A	91	THR
1	A	100	ARG
1	A	101	ARG
1	A	102	ARG
1	A	103	ASP
1	A	110	THR
1	A	120	ASN
1	A	142	GLU
1	A	158	ILE
1	A	166	GLU
1	A	178	ASP
1	A	180	TYR
1	A	209	LEU
1	A	212	ARG
1	A	213	LEU
1	A	240	VAL
1	A	242	LYS
1	A	245	LEU
1	A	250	VAL
1	A	260	ASP
1	A	263	LEU
1	A	282	ASN
1	A	287	HIS
1	A	294	PHE
1	A	323	LEU
1	A	335	GLN
1	A	338	SER
1	A	341	LEU
1	A	348	MET
1	A	355	ASP

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Mol	Chain	Res	Type
1	A	363	PHE
1	A	382	LYS
1	A	384	LEU
1	A	391	ASN
1	A	400	PHE
1	A	418	PHE
1	A	427	ASN
1	A	446	THR
1	A	484	ASN
1	A	488	CYS
1	A	507	LYS
1	A	523	ARG
1	A	525	SER
1	A	529	SER
1	A	535	ARG
1	A	546	THR
1	A	551	LEU
1	A	558	THR
1	A	561	THR
1	A	566	LEU
1	A	576	MET
1	A	584	THR
1	B	38	THR
1	B	42	LEU
1	B	44	ARG
1	B	48	VAL
1	B	59	ARG
1	B	70	LEU
1	B	85	GLN
1	B	89	LEU
1	B	101	ARG
1	B	102	ARG
1	B	107	ARG
1	B	125	ASP
1	B	131	LYS
1	B	192	ASP
1	B	196	TYR
1	B	197	MET
1	B	204	GLU
1	B	254	PHE
1	B	257	CYS
1	B	258	HIS

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Mol	Chain	Res	Type
1	B	264	THR
1	B	280	ASN
1	B	282	ASN
1	B	286	LYS
1	B	291	VAL
1	B	305	ASN
1	B	355	ASP
1	B	365	LEU
1	B	391	ASN
1	B	407	ILE
1	B	417	LEU
1	B	418	PHE
1	B	431	THR
1	B	434	VAL
1	B	454	ARG
1	B	463	GLU
1	B	478	ASP
1	B	483	LEU
1	B	484	ASN
1	B	489	LYS
1	B	491	ILE
1	B	505	SER
1	B	507	LYS
1	B	525	SER
1	B	527	THR
1	B	548	LYS
1	B	551	LEU
1	B	554	LYS
1	B	558	THR
1	B	561	THR
1	B	566	LEU
1	B	583	LYS
1	B	584	THR
1	C	30	TYR
1	C	31	THR
1	C	48	VAL
1	C	52	LEU
1	C	59	ARG
1	C	60	TYR
1	C	62	THR
1	C	67	GLN
1	C	110	THR

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Mol	Chain	Res	Type
1	C	130	ILE
1	C	131	LYS
1	C	143	LYS
1	C	160	MET
1	C	163	THR
1	C	166	GLU
1	C	179	ASP
1	C	180	TYR
1	C	196	TYR
1	C	203	PHE
1	C	209	LEU
1	C	232	ARG
1	C	254	PHE
1	C	260	ASP
1	C	263	LEU
1	C	278	ASP
1	C	288	ILE
1	C	290	THR
1	C	311	ARG
1	C	334	THR
1	C	335	GLN
1	C	348	MET
1	C	351	SER
1	C	385	TYR
1	C	388	LYS
1	C	390	PHE
1	C	391	ASN
1	C	409	GLU
1	C	418	PHE
1	C	431	THR
1	C	479	ASP
1	C	483	LEU
1	C	535	ARG
1	C	548	LYS
1	C	550	HIS
1	C	558	THR
1	C	561	THR
1	C	566	LEU
1	D	33	ASN
1	D	36	GLN
1	D	43	HIS
1	D	52	LEU

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Mol	Chain	Res	Type
1	D	61	TYR
1	D	79	ARG
1	D	108	LYS
1	D	110	THR
1	D	127	ASP
1	D	128	PHE
1	D	136	ASN
1	D	144	LEU
1	D	157	HIS
1	D	167	VAL
1	D	179	ASP
1	D	197	MET
1	D	203	PHE
1	D	212	ARG
1	D	242	LYS
1	D	253	ASP
1	D	258	HIS
1	D	273	MET
1	D	278	ASP
1	D	280	ASN
1	D	286	LYS
1	D	290	THR
1	D	304	ARG
1	D	320	LEU
1	D	370	THR
1	D	385	TYR
1	D	388	LYS
1	D	408	ARG
1	D	409	GLU
1	D	413	ILE
1	D	418	PHE
1	D	431	THR
1	D	470	ASP
1	D	476	VAL
1	D	483	LEU
1	D	497	THR
1	D	507	LYS
1	D	518	SER
1	D	520	PHE
1	D	522	LEU
1	D	541	TYR
1	D	547	VAL

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Mol	Chain	Res	Type
1	D	550	HIS
1	D	558	THR
1	D	563	LEU
1	D	564	LYS
1	D	566	LEU
1	D	577	GLU
1	D	582	ARG
1	D	586	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	282	ASN
1	B	36	GLN
1	B	40	ASN
1	B	262	ASN

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 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	565/592 (95%)	-0.04	26 (4%)	36	28	31, 65, 153, 257	0
1	B	559/592 (94%)	-0.25	10 (1%)	71	62	28, 62, 141, 198	0
1	C	561/592 (94%)	-0.05	20 (3%)	46	37	34, 66, 147, 223	0
1	D	559/592 (94%)	-0.01	20 (3%)	46	37	30, 71, 160, 250	0
All	All	2244/2368 (94%)	-0.09	76 (3%)	49	40	28, 66, 153, 257	0

All (76) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	478	ASP	6.9
1	A	549	SER	5.7
1	D	125	ASP	5.1
1	C	127	ASP	5.1
1	A	47	ALA	4.9
1	B	103	ASP	4.8
1	A	547	VAL	4.8
1	D	120	ASN	4.7
1	C	336	SER	4.6
1	C	387	GLY	4.6
1	B	123	GLY	4.5
1	D	550	HIS	4.5
1	A	46	GLY	4.4
1	D	553	GLU	4.3
1	A	25	PHE	4.2
1	D	386	GLY	4.2
1	D	528	GLY	3.9
1	B	265	TYR	3.9
1	C	286	LYS	3.9
1	A	29	ASN	3.8
1	C	120	ASN	3.7

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Mol	Chain	Res	Type	RSRZ
1	C	121	PRO	3.6
1	A	548	LYS	3.5
1	A	265	TYR	3.4
1	A	550	HIS	3.3
1	B	117	ALA	3.3
1	C	265	TYR	3.3
1	C	530	SER	3.2
1	A	390	PHE	3.1
1	C	124	PRO	3.1
1	B	288	ILE	3.1
1	C	45	GLN	2.9
1	A	44	ARG	2.9
1	B	264	THR	2.9
1	C	546	THR	2.8
1	A	339	SER	2.8
1	D	456	ASP	2.8
1	D	483	LEU	2.8
1	A	26	GLN	2.7
1	D	180	TYR	2.6
1	C	550	HIS	2.6
1	D	48	VAL	2.6
1	B	557	PRO	2.6
1	C	551	LEU	2.6
1	A	336	SER	2.6
1	A	48	VAL	2.5
1	A	164	LEU	2.5
1	A	529	SER	2.4
1	C	126	ALA	2.4
1	A	157	HIS	2.3
1	A	337	SER	2.3
1	A	127	ASP	2.3
1	C	179	ASP	2.3
1	C	386	GLY	2.3
1	B	389	ASP	2.2
1	D	520	PHE	2.2
1	A	287	HIS	2.2
1	C	128	PHE	2.2
1	B	102	ARG	2.2
1	D	476	VAL	2.2
1	D	122	GLY	2.2
1	A	264	THR	2.2
1	D	527	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	122	GLY	2.2
1	D	566	LEU	2.2
1	A	481	PRO	2.1
1	C	123	GLY	2.1
1	D	546	THR	2.1
1	C	500	ILE	2.1
1	A	45	GLN	2.1
1	C	553	GLU	2.1
1	D	534	ILE	2.1
1	D	390	PHE	2.1
1	A	128	PHE	2.0
1	D	337	SER	2.0
1	D	126	ALA	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
2	MG	A	601	1/1	0.97	0.16	-	37,37,37,37	0
2	MG	D	601	1/1	0.99	0.26	-	19,19,19,19	0
2	MG	B	601	1/1	0.98	0.17	-	32,32,32,32	0
2	MG	C	601	1/1	0.97	0.15	-	29,29,29,29	0

6.5 Other polymers (i)

There are no such residues in this entry.