Full wwPDB X-ray Structure Validation Report ⓘ

Nov 2, 2023 – 03:36 PM EDT

PDB ID	:	3VGK
Title	:	Crystal structure of a ROK family glucokinase from Streptomyces griseus
Authors	:	Miyazono, K.; Tabei, N.; Morita, S.; Ohnishi, Y.; Horinouchi, S.; Tanokura, M.
Deposited on	:	2011-08-15
Resolution	:	3.25 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

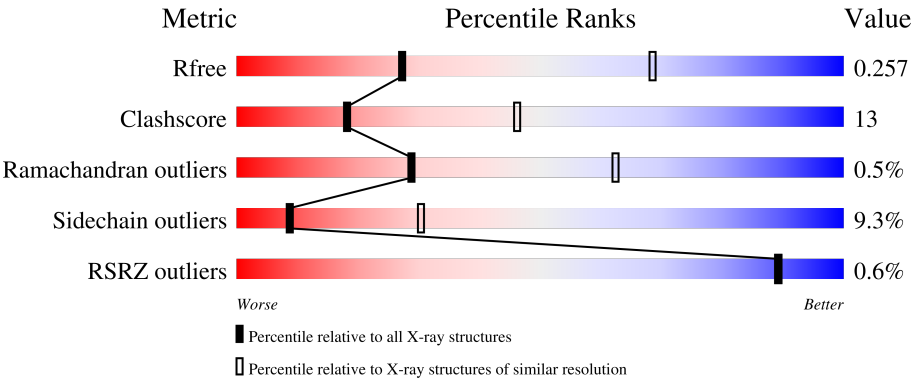
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 3.25 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	1191 (3.30-3.22)
Clashscore	141614	1251 (3.30-3.22)
Ramachandran outliers	138981	1229 (3.30-3.22)
Sidechain outliers	138945	1228 (3.30-3.22)
RSRZ outliers	127900	1154 (3.30-3.22)

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 of 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	321	73% 22%
1	B	321	% 70% 26%
1	C	321	70% 23%
1	D	321	65% 29%
1	E	321	% 68% 26%

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Mol	Chain	Length	Quality of chain
1	F	321	72% 24%
1	G	321	65% 29%
1	H	321	2% 63% 30%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 18142 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 Glucokinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	311	Total	C	N	O	S	0	0	0
			2267	1420	414	428	5			
1	B	312	Total	C	N	O	S	0	0	0
			2271	1422	415	429	5			
1	C	310	Total	C	N	O	S	0	0	0
			2263	1418	413	427	5			
1	D	311	Total	C	N	O	S	0	0	0
			2267	1420	414	428	5			
1	E	310	Total	C	N	O	S	0	0	0
			2263	1418	413	427	5			
1	F	310	Total	C	N	O	S	0	0	0
			2263	1418	413	427	5			
1	G	311	Total	C	N	O	S	0	0	0
			2267	1420	414	428	5			
1	H	310	Total	C	N	O	S	0	0	0
			2263	1418	413	427	5			

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	314	LEU	-	expression tag	UNP B1VZT1
A	315	GLU	-	expression tag	UNP B1VZT1
A	316	HIS	-	expression tag	UNP B1VZT1
A	317	HIS	-	expression tag	UNP B1VZT1
A	318	HIS	-	expression tag	UNP B1VZT1
A	319	HIS	-	expression tag	UNP B1VZT1
A	320	HIS	-	expression tag	UNP B1VZT1
A	321	HIS	-	expression tag	UNP B1VZT1
B	314	LEU	-	expression tag	UNP B1VZT1
B	315	GLU	-	expression tag	UNP B1VZT1
B	316	HIS	-	expression tag	UNP B1VZT1
B	317	HIS	-	expression tag	UNP B1VZT1
B	318	HIS	-	expression tag	UNP B1VZT1

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Chain	Residue	Modelled	Actual	Comment	Reference
B	319	HIS	-	expression tag	UNP B1VZT1
B	320	HIS	-	expression tag	UNP B1VZT1
B	321	HIS	-	expression tag	UNP B1VZT1
C	314	LEU	-	expression tag	UNP B1VZT1
C	315	GLU	-	expression tag	UNP B1VZT1
C	316	HIS	-	expression tag	UNP B1VZT1
C	317	HIS	-	expression tag	UNP B1VZT1
C	318	HIS	-	expression tag	UNP B1VZT1
C	319	HIS	-	expression tag	UNP B1VZT1
C	320	HIS	-	expression tag	UNP B1VZT1
C	321	HIS	-	expression tag	UNP B1VZT1
D	314	LEU	-	expression tag	UNP B1VZT1
D	315	GLU	-	expression tag	UNP B1VZT1
D	316	HIS	-	expression tag	UNP B1VZT1
D	317	HIS	-	expression tag	UNP B1VZT1
D	318	HIS	-	expression tag	UNP B1VZT1
D	319	HIS	-	expression tag	UNP B1VZT1
D	320	HIS	-	expression tag	UNP B1VZT1
D	321	HIS	-	expression tag	UNP B1VZT1
E	314	LEU	-	expression tag	UNP B1VZT1
E	315	GLU	-	expression tag	UNP B1VZT1
E	316	HIS	-	expression tag	UNP B1VZT1
E	317	HIS	-	expression tag	UNP B1VZT1
E	318	HIS	-	expression tag	UNP B1VZT1
E	319	HIS	-	expression tag	UNP B1VZT1
E	320	HIS	-	expression tag	UNP B1VZT1
E	321	HIS	-	expression tag	UNP B1VZT1
F	314	LEU	-	expression tag	UNP B1VZT1
F	315	GLU	-	expression tag	UNP B1VZT1
F	316	HIS	-	expression tag	UNP B1VZT1
F	317	HIS	-	expression tag	UNP B1VZT1
F	318	HIS	-	expression tag	UNP B1VZT1
F	319	HIS	-	expression tag	UNP B1VZT1
F	320	HIS	-	expression tag	UNP B1VZT1
F	321	HIS	-	expression tag	UNP B1VZT1
G	314	LEU	-	expression tag	UNP B1VZT1
G	315	GLU	-	expression tag	UNP B1VZT1
G	316	HIS	-	expression tag	UNP B1VZT1
G	317	HIS	-	expression tag	UNP B1VZT1
G	318	HIS	-	expression tag	UNP B1VZT1
G	319	HIS	-	expression tag	UNP B1VZT1
G	320	HIS	-	expression tag	UNP B1VZT1

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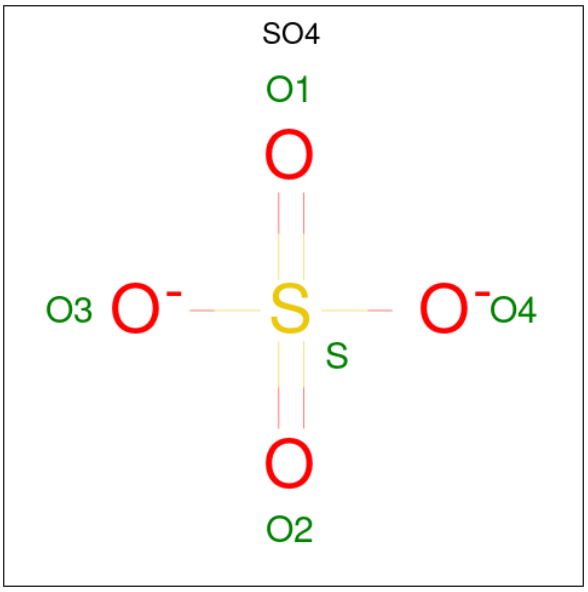
Chain	Residue	Modelled	Actual	Comment	Reference
G	321	HIS	-	expression tag	UNP B1VZT1
H	314	LEU	-	expression tag	UNP B1VZT1
H	315	GLU	-	expression tag	UNP B1VZT1
H	316	HIS	-	expression tag	UNP B1VZT1
H	317	HIS	-	expression tag	UNP B1VZT1
H	318	HIS	-	expression tag	UNP B1VZT1
H	319	HIS	-	expression tag	UNP B1VZT1
H	320	HIS	-	expression tag	UNP B1VZT1
H	321	HIS	-	expression tag	UNP B1VZT1

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Zn 1 1	0	0
2	B	1	Total Zn 1 1	0	0
2	C	1	Total Zn 1 1	0	0
2	D	1	Total Zn 1 1	0	0
2	E	1	Total Zn 1 1	0	0
2	F	1	Total Zn 1 1	0	0
2	G	1	Total Zn 1 1	0	0
2	H	1	Total Zn 1 1	0	0

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



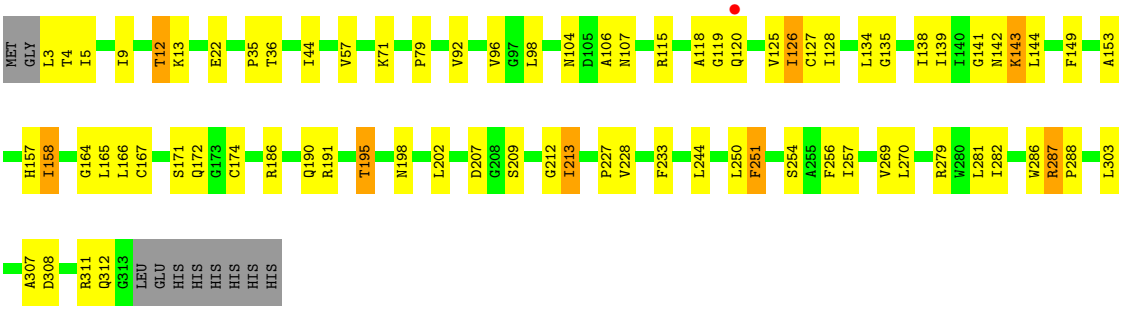
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total O S 5 4 1	0	0
3	E	1	Total O S 5 4 1	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

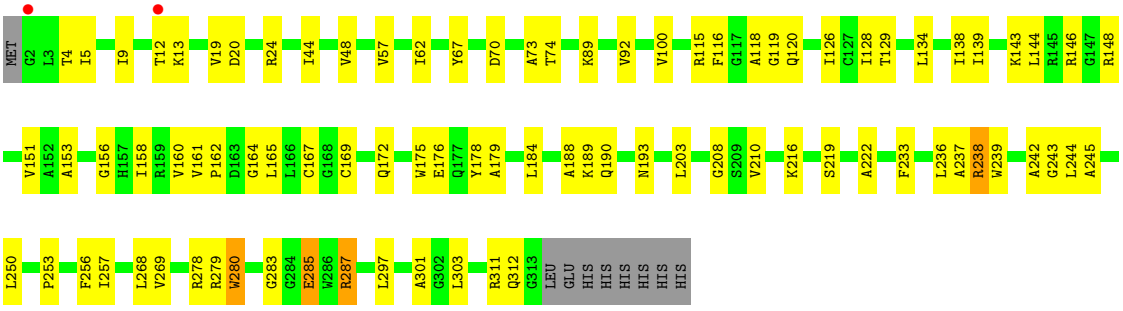
• Molecule 1: Glucokinase

Chain A:



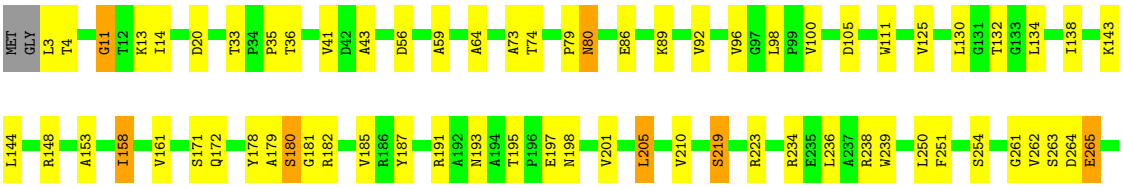
• Molecule 1: Glucokinase

Chain B:



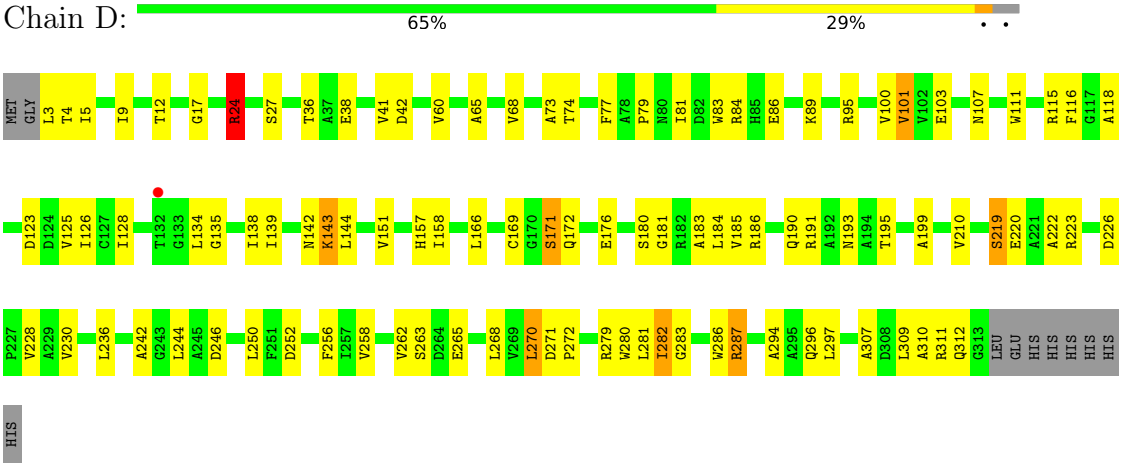
• Molecule 1: Glucokinase

Chain C:



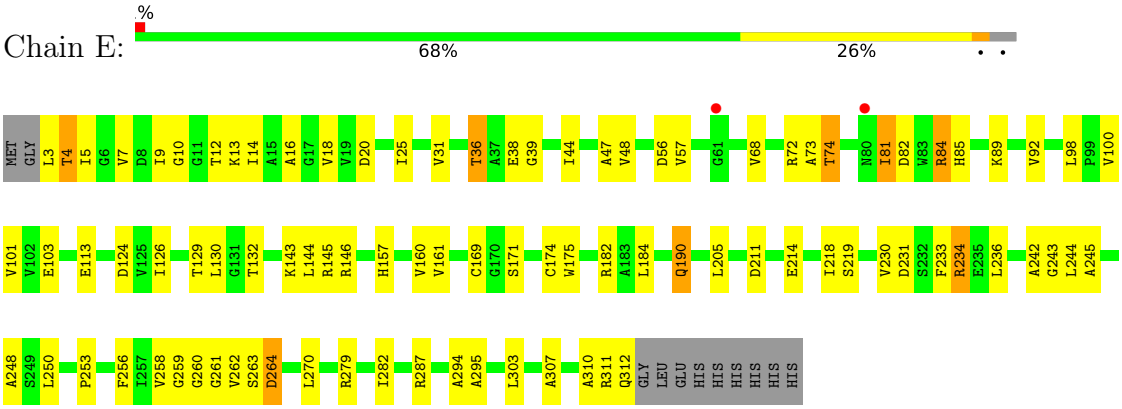
• Molecule 1: Glucokinase

Chain D:



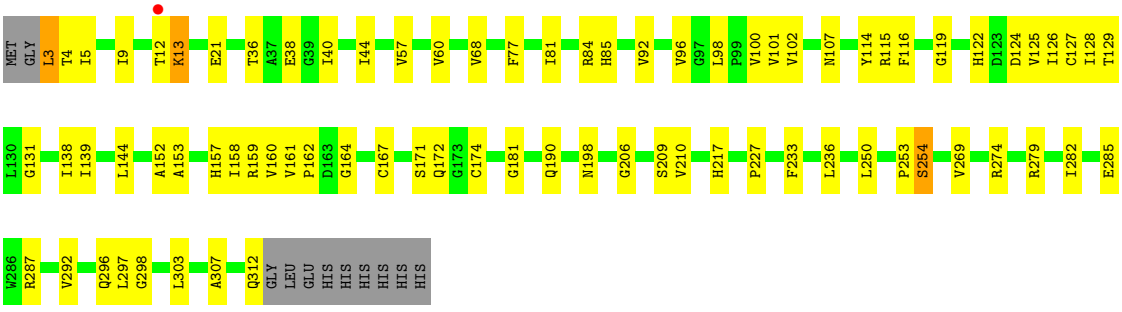
• Molecule 1: Glucokinase

Chain E:



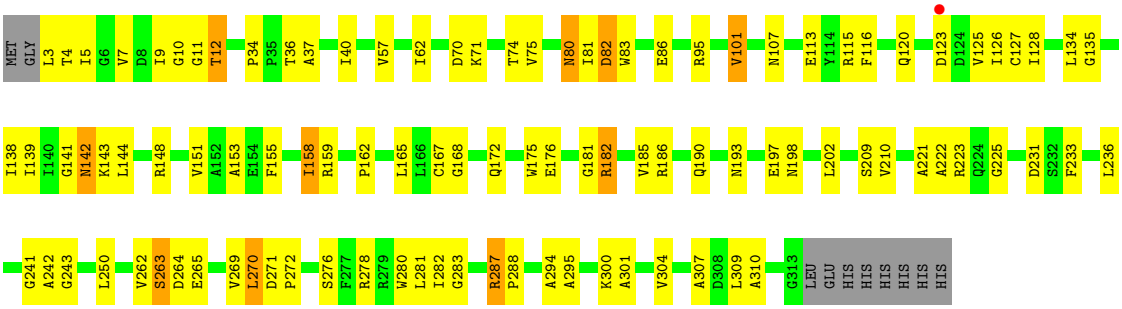
• Molecule 1: Glucokinase

Chain F:



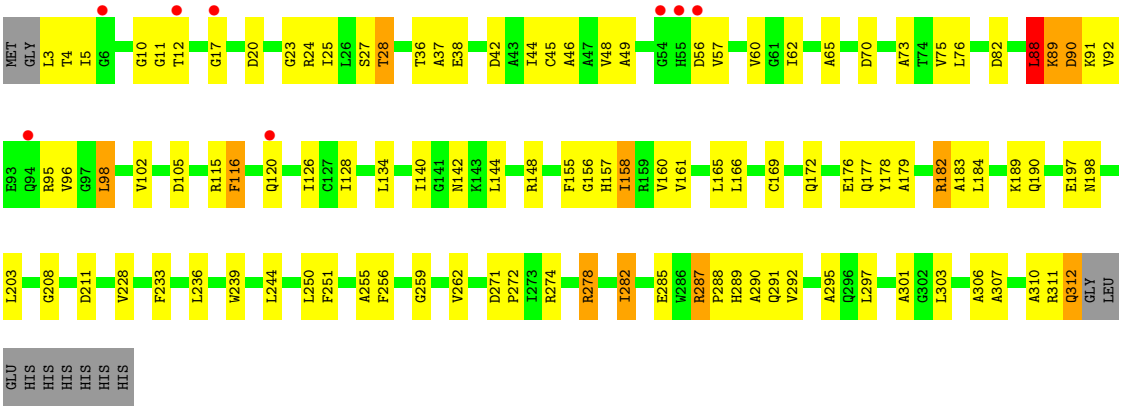
• Molecule 1: Glucokinase

Chain G:



• Molecule 1: Glucokinase

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	98.69Å 173.70Å 124.03Å 90.00° 106.69° 90.00°	Depositor
Resolution (Å)	20.00 – 3.25 19.67 – 3.25	Depositor EDS
% Data completeness (in resolution range)	96.8 (20.00-3.25) 96.8 (19.67-3.25)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.28 (at 3.22Å)	Xtriage
Refinement program	REFMAC refmac_5.5.0109	Depositor
R, R_{free}	0.206 , 0.264 0.205 , 0.257	Depositor DCC
R_{free} test set	6121 reflections (10.08%)	wwPDB-VP
Wilson B-factor (Å^2)	87.4	Xtriage
Anisotropy	0.091	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 31.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	18142	wwPDB-VP
Average B, all atoms (Å^2)	87.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 25.97 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.8729e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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: ZN, SO4

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	0.70	0/2308	0.74	0/3129
1	B	0.69	0/2312	0.73	0/3134
1	C	0.66	0/2304	0.72	0/3124
1	D	0.71	0/2308	0.76	1/3129 (0.0%)
1	E	0.70	0/2304	0.76	0/3124
1	F	0.69	0/2304	0.73	0/3124
1	G	0.70	0/2308	0.78	1/3129 (0.0%)
1	H	0.63	0/2304	0.71	0/3124
All	All	0.68	0/18452	0.74	2/25017 (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	D	24	ARG	NE-CZ-NH2	5.96	123.28	120.30
1	G	278	ARG	NE-CZ-NH2	5.62	123.11	120.30

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	2267	0	2237	49	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2271	0	2241	65	0
1	C	2263	0	2234	57	0
1	D	2267	0	2237	76	0
1	E	2263	0	2234	61	0
1	F	2263	0	2234	53	0
1	G	2267	0	2237	80	0
1	H	2263	0	2234	83	0
2	A	1	0	0	0	0
2	B	1	0	0	1	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
3	B	5	0	0	0	0
3	E	5	0	0	0	0
All	All	18142	0	17888	482	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 13.

All (482) 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:C:193:ASN:HD22	1:C:210:VAL:HG21	1.22	1.02
1:G:270:LEU:CD1	1:G:294:ALA:HB2	1.96	0.96
1:G:270:LEU:HD13	1:G:294:ALA:HB2	1.46	0.94
1:B:172:GLN:HE21	1:H:190:GLN:HE22	1.16	0.94
1:B:167:CYS:HG	2:B:322:ZN:ZN	0.69	0.88
1:B:190:GLN:HE22	1:H:172:GLN:HE21	1.22	0.87
1:D:270:LEU:HD13	1:D:294:ALA:HB2	1.56	0.86
1:G:101:VAL:HG21	1:G:310:ALA:HA	1.56	0.85
1:B:190:GLN:NE2	1:H:172:GLN:HE21	1.75	0.85
1:F:190:GLN:HE22	1:G:172:GLN:HE21	1.21	0.84
1:H:255:ALA:HB1	1:H:291:GLN:O	1.77	0.84
1:B:126:ILE:HD13	1:B:253:PRO:HG3	1.59	0.84
1:E:129:THR:HG22	1:E:260:GLY:H	1.40	0.83
1:B:5:ILE:HG13	1:B:57:VAL:HG11	1.59	0.82
1:H:255:ALA:HA	1:H:290:ALA:HB1	1.60	0.82
1:C:193:ASN:ND2	1:C:210:VAL:HG21	1.95	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:190:GLN:NE2	1:G:172:GLN:HE21	1.79	0.80
1:B:44:ILE:O	1:B:48:VAL:HG23	1.84	0.78
1:A:190:GLN:HE22	1:D:172:GLN:HE21	1.29	0.77
1:C:92:VAL:HG12	1:C:100:VAL:HG21	1.67	0.77
1:B:92:VAL:HG12	1:B:100:VAL:HG21	1.67	0.77
1:H:5:ILE:HB	1:H:60:VAL:HG22	1.67	0.76
1:D:244:LEU:HD22	1:D:256:PHE:CD1	2.20	0.76
1:H:73:ALA:HA	1:H:89:LYS:HG2	1.67	0.75
1:D:158:ILE:HG21	1:F:250:LEU:HD21	1.67	0.75
1:A:143:LYS:HA	1:A:143:LYS:HE2	1.69	0.74
1:C:59:ALA:HB1	1:C:310:ALA:HB1	1.68	0.74
1:E:4:THR:CG2	1:E:307:ALA:HB1	2.18	0.74
1:H:65:ALA:HA	1:H:105:ASP:OD1	1.88	0.74
1:D:270:LEU:CD1	1:D:294:ALA:HB2	2.18	0.73
1:G:34:PRO:HD2	1:G:40:ILE:HD13	1.69	0.73
1:G:134:LEU:HD23	1:G:135:GLY:N	2.04	0.73
1:F:190:GLN:HE22	1:G:172:GLN:NE2	1.87	0.72
1:E:4:THR:HG23	1:E:307:ALA:HB1	1.72	0.72
1:B:9:ILE:HD11	1:B:44:ILE:HD11	1.72	0.71
1:E:68:VAL:HG13	1:E:74:THR:O	1.90	0.71
1:F:107:ASN:HB3	1:F:144:LEU:HD21	1.73	0.71
1:B:116:PHE:HB2	1:B:297:LEU:HD11	1.73	0.71
1:E:5:ILE:HD12	1:E:48:VAL:HG13	1.74	0.69
1:D:74:THR:HG23	1:D:86:GLU:O	1.93	0.69
1:C:111:TRP:CG	1:C:309:LEU:HD21	2.28	0.69
1:G:281:LEU:HD12	1:G:282:ILE:H	1.57	0.68
1:E:250:LEU:HD21	1:H:158:ILE:HG21	1.73	0.68
1:H:128:ILE:HD13	1:H:244:LEU:HD21	1.75	0.68
1:C:138:ILE:HD13	1:C:251:PHE:CE1	2.29	0.67
1:G:233:PHE:CE1	1:G:269:VAL:HG22	2.28	0.67
1:A:303:LEU:C	1:A:303:LEU:HD23	2.15	0.67
1:C:303:LEU:C	1:C:303:LEU:HD23	2.15	0.67
1:A:172:GLN:NE2	1:D:186:ARG:HE	1.93	0.66
1:H:203:LEU:HD22	1:H:208:GLY:O	1.95	0.66
1:G:101:VAL:CG2	1:G:310:ALA:HA	2.23	0.66
1:H:92:VAL:HG12	1:H:92:VAL:O	1.95	0.66
1:F:160:VAL:HG23	1:F:161:VAL:HG23	1.77	0.66
1:C:238:ARG:HG3	1:C:280:TRP:CH2	2.31	0.66
1:C:172:GLN:HE21	1:E:190:GLN:HE22	1.45	0.65
1:G:270:LEU:HD11	1:G:294:ALA:HB2	1.75	0.65
1:D:138:ILE:C	1:D:139:ILE:HD12	2.17	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:236:LEU:O	1:F:236:LEU:HD23	1.97	0.65
1:F:274:ARG:HG3	1:F:292:VAL:HB	1.79	0.65
1:A:138:ILE:HG13	1:A:153:ALA:HB2	1.76	0.65
1:G:37:ALA:HB2	1:G:82:ASP:OD1	1.98	0.64
1:H:88:LEU:HD13	1:H:88:LEU:C	2.17	0.64
1:E:184:LEU:HD13	1:E:236:LEU:HD12	1.78	0.64
1:G:134:LEU:HD23	1:G:134:LEU:C	2.17	0.64
1:B:283:GLY:O	1:B:287:ARG:HG3	1.98	0.64
1:F:126:ILE:HD13	1:F:253:PRO:HB3	1.80	0.64
1:F:303:LEU:C	1:F:303:LEU:HD23	2.17	0.64
1:G:80:ASN:N	1:G:80:ASN:HD22	1.93	0.64
1:A:250:LEU:HD13	1:G:250:LEU:HD13	1.79	0.63
1:D:222:ALA:HB3	1:D:268:LEU:HD21	1.80	0.63
1:H:184:LEU:HD13	1:H:236:LEU:HD12	1.80	0.63
1:C:4:THR:HG23	1:C:307:ALA:HB1	1.81	0.63
1:B:160:VAL:HG23	1:B:161:VAL:HG23	1.81	0.63
1:B:190:GLN:HE22	1:H:172:GLN:NE2	1.95	0.63
1:A:233:PHE:CE1	1:A:269:VAL:HG22	2.34	0.63
1:B:250:LEU:HD21	1:C:158:ILE:HG21	1.79	0.63
1:H:155:PHE:O	1:H:158:ILE:HG23	1.99	0.63
1:E:81:ILE:HG22	1:E:82:ASP:H	1.65	0.62
1:B:4:THR:HG22	1:B:311:ARG:NH2	2.14	0.62
1:E:259:GLY:O	1:E:263:SER:HB3	2.00	0.62
1:E:160:VAL:HG23	1:E:161:VAL:HG23	1.82	0.61
1:G:4:THR:HG23	1:G:307:ALA:HB1	1.81	0.61
1:H:96:VAL:CG2	1:H:98:LEU:HD12	2.30	0.61
1:A:9:ILE:HD11	1:A:44:ILE:HD11	1.83	0.61
1:C:303:LEU:HD23	1:C:303:LEU:O	2.00	0.61
1:D:139:ILE:HD12	1:D:139:ILE:N	2.16	0.61
1:G:155:PHE:O	1:G:158:ILE:HG23	2.01	0.61
1:H:128:ILE:HD13	1:H:244:LEU:CD2	2.30	0.61
1:E:230:VAL:HG12	1:E:234:ARG:HD2	1.83	0.60
1:C:270:LEU:HD13	1:C:294:ALA:HB2	1.82	0.60
1:C:92:VAL:CG1	1:C:100:VAL:HG21	2.31	0.60
1:E:25:ILE:H	1:E:25:ILE:HD12	1.66	0.60
1:B:237:ALA:O	1:B:238:ARG:C	2.40	0.60
1:C:59:ALA:CB	1:C:310:ALA:HB1	2.30	0.60
1:E:145:ARG:HH11	1:H:140:ILE:HG22	1.65	0.60
1:F:172:GLN:NE2	1:G:186:ARG:HE	1.99	0.60
1:G:4:THR:CG2	1:G:307:ALA:HB1	2.32	0.60
1:F:152:ALA:O	1:F:153:ALA:HB3	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:88:LEU:C	1:H:88:LEU:CD1	2.70	0.60
1:F:96:VAL:HG23	1:F:98:LEU:H	1.67	0.59
1:F:138:ILE:C	1:F:139:ILE:HD12	2.23	0.59
1:H:17:GLY:HA3	1:H:303:LEU:HD21	1.85	0.59
1:A:127:CYS:C	1:A:128:ILE:HD12	2.23	0.59
1:B:128:ILE:HD13	1:B:244:LEU:HD21	1.84	0.59
1:G:75:VAL:HG11	1:G:83:TRP:CE3	2.37	0.59
1:C:201:VAL:O	1:C:205:LEU:HD12	2.01	0.59
1:D:101:VAL:HG21	1:D:310:ALA:HA	1.84	0.59
1:A:92:VAL:O	1:A:96:VAL:HG22	2.02	0.59
1:B:92:VAL:CG1	1:B:100:VAL:HG21	2.31	0.59
1:B:233:PHE:CE1	1:B:269:VAL:HG22	2.37	0.59
1:H:88:LEU:HD12	1:H:102:VAL:CG2	2.33	0.59
1:E:250:LEU:HD13	1:H:250:LEU:HD13	1.85	0.58
1:C:181:GLY:O	1:C:185:VAL:HG23	2.03	0.58
1:H:311:ARG:O	1:H:312:GLN:HB2	2.03	0.58
1:D:250:LEU:HD13	1:F:250:LEU:CD1	2.33	0.58
1:D:271:ASP:HB3	1:D:272:PRO:HD3	1.85	0.58
1:D:118:ALA:HA	1:D:296:GLN:HE22	1.68	0.58
1:G:134:LEU:H	1:G:176:GLU:HG3	1.68	0.58
1:G:270:LEU:CD1	1:G:294:ALA:CB	2.78	0.58
1:H:17:GLY:HA2	1:H:28:THR:HG23	1.85	0.58
1:C:20:ASP:OD1	1:C:20:ASP:C	2.42	0.58
1:A:254:SER:HB3	1:G:148:ARG:HG2	1.84	0.57
1:H:37:ALA:HB2	1:H:82:ASP:HB3	1.87	0.57
1:D:111:TRP:CG	1:D:309:LEU:HD21	2.39	0.57
1:C:138:ILE:HG13	1:C:153:ALA:HB2	1.86	0.57
1:B:44:ILE:HD13	1:B:62:ILE:HD13	1.86	0.56
1:G:116:PHE:HA	1:G:120:GLN:HE21	1.70	0.56
1:F:68:VAL:HG11	1:F:102:VAL:O	2.06	0.56
1:A:139:ILE:N	1:A:139:ILE:HD12	2.20	0.56
1:B:236:LEU:HD23	1:B:236:LEU:C	2.26	0.56
1:D:258:VAL:HG12	1:D:263:SER:OG	2.05	0.56
1:C:311:ARG:O	1:C:312:GLN:HB2	2.05	0.56
1:F:159:ARG:HD2	1:F:162:PRO:HA	1.88	0.56
1:G:181:GLY:O	1:G:185:VAL:HG23	2.05	0.56
1:G:263:SER:C	1:G:265:GLU:H	2.08	0.56
1:E:113:GLU:OE2	1:E:295:ALA:HB1	2.06	0.55
1:D:199:ALA:HB2	1:D:228:VAL:HG21	1.86	0.55
1:E:282:ILE:HD13	1:H:157:HIS:HB3	1.88	0.55
1:D:42:ASP:OD1	1:D:95:ARG:NH1	2.34	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:12:THR:HG23	1:E:13:LYS:HG2	1.89	0.55
1:C:261:GLY:O	1:C:264:ASP:HB2	2.06	0.55
1:F:131:GLY:O	1:F:181:GLY:N	2.35	0.55
1:E:245:ALA:O	1:E:248:ALA:HB3	2.06	0.55
1:G:141:GLY:O	1:G:142:ASN:HB2	2.06	0.55
1:D:181:GLY:O	1:D:185:VAL:HG23	2.07	0.55
1:D:226:ASP:O	1:D:230:VAL:HG23	2.07	0.55
1:D:134:LEU:HD23	1:D:135:GLY:N	2.22	0.54
1:E:9:ILE:HG23	1:E:14:ILE:HG12	1.89	0.54
1:B:118:ALA:HB3	1:B:257:ILE:CD1	2.37	0.54
1:B:12:THR:HG23	1:B:13:LYS:CG	2.38	0.54
1:B:126:ILE:HD13	1:B:253:PRO:CG	2.35	0.54
1:H:37:ALA:CB	1:H:82:ASP:HB3	2.38	0.54
1:A:118:ALA:HB3	1:A:257:ILE:HD13	1.90	0.54
1:C:111:TRP:CD1	1:C:309:LEU:CD2	2.92	0.54
1:B:238:ARG:HG3	1:B:280:TRP:CH2	2.43	0.53
1:G:141:GLY:O	1:G:142:ASN:CB	2.55	0.53
1:B:167:CYS:SG	1:B:169:CYS:SG	3.06	0.53
1:D:158:ILE:HG21	1:F:250:LEU:CD2	2.37	0.53
1:C:134:LEU:HD12	1:C:179:ALA:O	2.08	0.53
1:F:60:VAL:HB	1:F:100:VAL:HG22	1.90	0.53
1:H:197:GLU:HG2	1:H:198:ASN:ND2	2.22	0.53
1:H:57:VAL:HG12	1:H:98:LEU:HD22	1.89	0.53
1:C:74:THR:HG23	1:C:86:GLU:O	2.09	0.53
1:D:180:SER:O	1:D:183:ALA:HB3	2.08	0.53
1:G:262:VAL:O	1:G:262:VAL:CG1	2.57	0.53
1:D:169:CYS:SG	1:D:171:SER:HB2	2.49	0.53
1:G:222:ALA:O	1:G:225:GLY:N	2.33	0.53
1:D:286:TRP:CE2	1:F:77:PHE:CD1	2.97	0.53
1:B:9:ILE:CD1	1:B:44:ILE:HD11	2.37	0.53
1:B:237:ALA:O	1:B:239:TRP:N	2.42	0.53
1:C:197:GLU:HG2	1:C:198:ASN:ND2	2.24	0.53
1:A:107:ASN:HB3	1:A:144:LEU:HD21	1.91	0.53
1:B:172:GLN:HE21	1:H:190:GLN:NE2	1.97	0.53
1:B:172:GLN:NE2	1:H:190:GLN:HE22	1.97	0.52
1:B:128:ILE:HD13	1:B:244:LEU:CD2	2.40	0.52
1:C:144:LEU:HD22	1:C:309:LEU:HD11	1.91	0.52
1:H:75:VAL:HG12	1:H:75:VAL:O	2.08	0.52
1:E:303:LEU:C	1:E:303:LEU:HD23	2.29	0.52
1:C:236:LEU:C	1:C:236:LEU:HD23	2.30	0.52
1:D:307:ALA:O	1:D:310:ALA:HB3	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:12:THR:HG23	1:B:13:LYS:HG3	1.92	0.52
1:D:270:LEU:CD1	1:D:294:ALA:CB	2.86	0.52
1:E:282:ILE:CD1	1:H:157:HIS:HB3	2.40	0.52
1:F:164:GLY:O	1:F:172:GLN:HB3	2.10	0.52
1:G:182:ARG:HH11	1:G:182:ARG:HB2	1.74	0.52
1:G:270:LEU:HD11	1:G:294:ALA:CB	2.40	0.52
1:H:73:ALA:CA	1:H:89:LYS:HG2	2.36	0.52
1:A:9:ILE:CD1	1:A:44:ILE:HD11	2.40	0.52
1:F:157:HIS:HA	1:F:174:CYS:HB3	1.92	0.52
1:A:202:LEU:HD21	1:A:213:ILE:HG21	1.91	0.51
1:C:111:TRP:CD1	1:C:309:LEU:HD23	2.45	0.51
1:D:4:THR:HG22	1:D:311:ARG:NH2	2.24	0.51
1:G:127:CYS:C	1:G:128:ILE:HD12	2.30	0.51
1:G:139:ILE:HG23	1:G:143:LYS:O	2.10	0.51
1:B:175:TRP:CZ2	1:B:243:GLY:HA3	2.45	0.51
1:A:303:LEU:HD23	1:A:303:LEU:O	2.10	0.51
1:A:308:ASP:OD1	1:A:311:ARG:NH1	2.43	0.51
1:C:172:GLN:HE21	1:E:190:GLN:NE2	2.06	0.51
1:E:92:VAL:HG12	1:E:100:VAL:HG21	1.92	0.51
1:D:9:ILE:O	1:D:9:ILE:HG22	2.10	0.51
1:D:68:VAL:HG21	1:D:103:GLU:C	2.31	0.51
1:G:151:VAL:HG12	1:G:151:VAL:O	2.11	0.51
1:H:91:LYS:O	1:H:95:ARG:HG3	2.10	0.51
1:E:234:ARG:CB	1:E:234:ARG:HH21	2.23	0.51
1:A:134:LEU:HD23	1:A:135:GLY:N	2.25	0.51
1:G:80:ASN:N	1:G:80:ASN:ND2	2.58	0.51
1:D:128:ILE:HD13	1:D:244:LEU:HD21	1.93	0.51
1:F:206:GLY:HA2	1:F:217:HIS:CE1	2.45	0.51
1:D:116:PHE:HB2	1:D:297:LEU:HD11	1.92	0.50
1:D:157:HIS:CE1	1:D:169:CYS:HB3	2.46	0.50
1:D:286:TRP:CE2	1:F:77:PHE:HD1	2.29	0.50
1:G:125:VAL:C	1:G:126:ILE:HD12	2.31	0.50
1:G:283:GLY:O	1:G:287:ARG:HG3	2.11	0.50
1:B:242:ALA:O	1:B:245:ALA:HB3	2.11	0.50
1:G:271:ASP:HB3	1:G:272:PRO:HD3	1.94	0.50
1:B:138:ILE:C	1:B:139:ILE:HD12	2.32	0.50
1:D:125:VAL:C	1:D:126:ILE:HD12	2.31	0.50
1:C:303:LEU:C	1:C:303:LEU:CD2	2.80	0.50
1:A:244:LEU:HD22	1:A:256:PHE:CD1	2.47	0.50
1:D:183:ALA:O	1:D:184:LEU:C	2.48	0.50
1:D:283:GLY:O	1:D:287:ARG:HG3	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:20:ASP:OD1	1:E:20:ASP:C	2.50	0.50
1:B:285:GLU:CD	1:B:285:GLU:H	2.15	0.49
1:F:5:ILE:HG13	1:F:57:VAL:HG11	1.93	0.49
1:D:123:ASP:HA	1:D:142:ASN:ND2	2.27	0.49
1:F:233:PHE:CD1	1:F:269:VAL:HG22	2.48	0.49
1:E:57:VAL:HG12	1:E:98:LEU:HD13	1.95	0.49
1:H:177:GLN:HE22	1:H:182:ARG:CD	2.25	0.49
1:G:9:ILE:HD11	1:G:62:ILE:CG2	2.43	0.49
1:H:70:ASP:HB3	1:H:148:ARG:O	2.13	0.49
1:F:139:ILE:HD12	1:F:139:ILE:N	2.26	0.49
1:E:259:GLY:O	1:E:263:SER:CB	2.60	0.49
1:C:111:TRP:CG	1:C:309:LEU:CD2	2.94	0.49
1:E:157:HIS:HA	1:E:174:CYS:HB3	1.94	0.49
1:F:40:ILE:HD12	1:F:81:ILE:HG23	1.94	0.49
1:H:88:LEU:HD13	1:H:88:LEU:O	2.12	0.49
1:E:157:HIS:CE1	1:E:169:CYS:HB3	2.48	0.48
1:H:62:ILE:HD13	1:H:88:LEU:HD11	1.95	0.48
1:H:96:VAL:HG23	1:H:98:LEU:HD12	1.95	0.48
1:C:161:VAL:HG12	1:C:161:VAL:O	2.13	0.48
1:D:193:ASN:ND2	1:D:210:VAL:HG21	2.29	0.48
1:G:128:ILE:HD12	1:G:128:ILE:N	2.28	0.48
1:H:259:GLY:HA2	1:H:295:ALA:HB3	1.95	0.48
1:A:303:LEU:C	1:A:303:LEU:CD2	2.82	0.48
1:B:5:ILE:HG13	1:B:57:VAL:CG1	2.39	0.48
1:F:125:VAL:C	1:F:126:ILE:HD12	2.33	0.48
1:F:198:ASN:HD22	1:F:227:PRO:HG2	1.78	0.48
1:A:198:ASN:HB3	1:A:227:PRO:HB2	1.95	0.48
1:D:60:VAL:HB	1:D:100:VAL:HG22	1.96	0.48
1:E:311:ARG:O	1:E:312:GLN:HB2	2.14	0.48
1:G:281:LEU:HD12	1:G:282:ILE:N	2.27	0.48
1:H:157:HIS:ND1	1:H:169:CYS:HB3	2.29	0.48
1:F:114:TYR:HA	1:F:119:GLY:HA3	1.96	0.48
1:H:255:ALA:CB	1:H:291:GLN:O	2.57	0.48
1:G:107:ASN:HB3	1:G:144:LEU:HD21	1.96	0.48
1:A:172:GLN:HG3	1:D:190:GLN:HE22	1.79	0.48
1:C:273:ILE:O	1:C:274:ARG:C	2.52	0.48
1:C:64:ALA:O	1:C:105:ASP:N	2.47	0.47
1:G:34:PRO:CD	1:G:40:ILE:HD13	2.43	0.47
1:H:134:LEU:HD12	1:H:179:ALA:O	2.14	0.47
1:H:282:ILE:HD12	1:H:282:ILE:H	1.80	0.47
1:F:172:GLN:HE21	1:G:190:GLN:HE22	1.61	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:138:ILE:HG13	1:G:153:ALA:HB2	1.96	0.47
1:H:44:ILE:O	1:H:48:VAL:HG23	2.15	0.47
1:A:191:ARG:HB3	1:A:228:VAL:HG13	1.96	0.47
1:C:4:THR:HG21	1:C:307:ALA:O	2.15	0.47
1:G:134:LEU:C	1:G:134:LEU:CD2	2.82	0.47
1:A:164:GLY:O	1:A:172:GLN:HB3	2.15	0.47
1:E:57:VAL:HG12	1:E:98:LEU:CD1	2.45	0.47
1:E:72:ARG:NE	1:E:103:GLU:OE2	2.44	0.47
1:B:303:LEU:HD23	1:B:303:LEU:O	2.15	0.47
1:D:242:ALA:O	1:D:246:ASP:OD1	2.32	0.47
1:D:252:ASP:HB3	1:F:152:ALA:HB2	1.96	0.47
1:G:241:GLY:O	1:G:242:ALA:C	2.52	0.47
1:H:4:THR:HG23	1:H:307:ALA:HB1	1.96	0.47
1:H:23:GLY:HA3	1:H:116:PHE:CD1	2.50	0.47
1:A:125:VAL:C	1:A:126:ILE:HD12	2.35	0.47
1:B:203:LEU:HD22	1:B:208:GLY:O	2.15	0.47
1:D:286:TRP:CZ3	1:F:84:ARG:HG3	2.49	0.47
1:F:126:ILE:HG22	1:F:128:ILE:CD1	2.45	0.47
1:A:5:ILE:HG13	1:A:57:VAL:HG11	1.96	0.47
1:D:5:ILE:HA	1:D:17:GLY:O	2.15	0.47
1:D:236:LEU:HD23	1:D:236:LEU:C	2.35	0.47
1:E:250:LEU:CD1	1:H:250:LEU:HD13	2.45	0.47
1:H:244:LEU:HD22	1:H:256:PHE:CD1	2.50	0.47
1:B:119:GLY:N	1:B:257:ILE:HD11	2.30	0.46
1:E:5:ILE:HG12	1:E:18:VAL:HG22	1.97	0.46
1:A:195:THR:O	1:A:195:THR:OG1	2.25	0.46
1:D:134:LEU:H	1:D:176:GLU:CG	2.29	0.46
1:H:89:LYS:HG3	1:H:90:ASP:N	2.30	0.46
1:G:202:LEU:HD13	1:G:221:ALA:HB3	1.96	0.46
1:B:161:VAL:O	1:B:162:PRO:C	2.53	0.46
1:D:193:ASN:HD22	1:D:210:VAL:HG21	1.79	0.46
1:A:141:GLY:O	1:A:142:ASN:HB2	2.15	0.46
1:C:262:VAL:O	1:C:269:VAL:HG21	2.15	0.46
1:C:270:LEU:CD1	1:C:294:ALA:HB2	2.46	0.46
1:E:132:THR:CG2	1:E:182:ARG:NH2	2.79	0.46
1:H:184:LEU:HD21	1:H:233:PHE:CZ	2.51	0.46
1:G:82:ASP:OD1	1:G:82:ASP:O	2.34	0.46
1:D:65:ALA:O	1:D:79:PRO:HD2	2.15	0.46
1:E:175:TRP:CZ2	1:E:243:GLY:HA3	2.51	0.46
1:E:258:VAL:HB	1:E:270:LEU:HD21	1.97	0.46
1:G:193:ASN:HD22	1:G:210:VAL:HG11	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:236:LEU:HD23	1:G:236:LEU:C	2.36	0.46
1:C:187:TYR:O	1:C:191:ARG:HD2	2.16	0.46
1:C:219:SER:HB2	1:C:265:GLU:HG2	1.98	0.46
1:F:122:HIS:ND1	1:F:254:SER:OG	2.50	0.45
1:G:272:PRO:O	1:G:276:SER:N	2.48	0.45
1:H:156:GLY:O	1:H:176:GLU:HB2	2.15	0.45
1:H:92:VAL:O	1:H:92:VAL:CG1	2.63	0.45
1:B:19:VAL:HG12	1:B:20:ASP:O	2.16	0.45
1:D:111:TRP:CB	1:D:309:LEU:HD21	2.47	0.45
1:D:139:ILE:N	1:D:139:ILE:CD1	2.80	0.45
1:D:191:ARG:HB3	1:D:228:VAL:HG13	1.98	0.45
1:E:261:GLY:O	1:E:264:ASP:HB2	2.17	0.45
1:E:303:LEU:HD23	1:E:303:LEU:O	2.16	0.45
1:C:74:THR:HG23	1:C:86:GLU:C	2.37	0.45
1:A:287:ARG:HA	1:A:288:PRO:HD3	1.84	0.45
1:C:98:LEU:O	1:C:100:VAL:HG23	2.17	0.45
1:A:251:PHE:CD2	1:A:251:PHE:N	2.85	0.45
1:B:184:LEU:HD13	1:B:236:LEU:HB2	1.98	0.45
1:F:92:VAL:HG12	1:F:100:VAL:HG21	1.99	0.45
1:G:300:LYS:O	1:G:301:ALA:C	2.54	0.45
1:H:262:VAL:O	1:H:262:VAL:HG12	2.17	0.45
1:D:223:ARG:NH2	1:D:265:GLU:HG3	2.31	0.45
1:A:12:THR:HG23	1:A:13:LYS:HG2	1.98	0.45
1:C:14:ILE:HD12	1:C:43:ALA:CB	2.47	0.45
1:C:273:ILE:O	1:C:276:SER:N	2.50	0.45
1:D:286:TRP:NE1	1:F:77:PHE:CD1	2.84	0.45
1:A:138:ILE:O	1:A:144:LEU:HD12	2.17	0.45
1:A:157:HIS:HA	1:A:174:CYS:HB3	1.99	0.45
1:D:270:LEU:HD11	1:D:294:ALA:CB	2.46	0.45
1:D:271:ASP:HB3	1:D:272:PRO:CD	2.47	0.45
1:B:70:ASP:HB3	1:B:148:ARG:O	2.18	0.44
1:C:197:GLU:OE2	1:H:278:ARG:NH2	2.50	0.44
1:E:130:LEU:O	1:E:262:VAL:HG23	2.16	0.44
1:A:119:GLY:O	1:A:120:GLN:C	2.56	0.44
1:F:236:LEU:HD23	1:F:236:LEU:C	2.37	0.44
1:H:46:ALA:O	1:H:49:ALA:HB3	2.17	0.44
1:E:126:ILE:HD13	1:E:253:PRO:HG3	1.99	0.44
1:C:148:ARG:O	1:C:148:ARG:NH1	2.41	0.44
1:E:81:ILE:HG22	1:E:82:ASP:N	2.30	0.44
1:G:113:GLU:OE2	1:G:295:ALA:HB1	2.17	0.44
1:G:167:CYS:SG	1:G:168:GLY:N	2.90	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:92:VAL:O	1:H:96:VAL:HG22	2.17	0.44
1:H:297:LEU:HB2	1:H:301:ALA:HB2	2.00	0.44
1:A:167:CYS:HB3	1:A:171:SER:O	2.18	0.44
1:G:7:VAL:HB	1:G:62:ILE:HG23	1.99	0.44
1:H:178:TYR:HB3	1:H:239:TRP:CG	2.52	0.44
1:A:4:THR:HG21	1:A:307:ALA:O	2.17	0.44
1:A:4:THR:HG22	1:A:311:ARG:NH2	2.33	0.44
1:B:4:THR:CG2	1:B:311:ARG:NH2	2.81	0.44
1:C:223:ARG:HH22	1:C:265:GLU:HG3	1.81	0.44
1:E:44:ILE:O	1:E:48:VAL:HG23	2.18	0.44
1:G:125:VAL:O	1:G:126:ILE:HD12	2.18	0.44
1:H:287:ARG:HA	1:H:288:PRO:HD2	1.85	0.44
1:H:166:LEU:HD23	1:H:172:GLN:HG2	1.99	0.44
1:E:231:ASP:HA	1:E:234:ARG:HD3	2.00	0.44
1:H:96:VAL:HG23	1:H:98:LEU:H	1.83	0.44
1:C:73:ALA:HA	1:C:89:LYS:HB2	1.99	0.43
1:D:107:ASN:HB3	1:D:144:LEU:HD21	1.99	0.43
1:E:218:ILE:HG22	1:E:233:PHE:CE2	2.53	0.43
1:F:233:PHE:CE1	1:F:269:VAL:HG22	2.52	0.43
1:G:134:LEU:N	1:G:176:GLU:HG3	2.33	0.43
1:B:134:LEU:H	1:B:176:GLU:HG2	1.83	0.43
1:C:132:THR:HG22	1:C:182:ARG:HD3	2.00	0.43
1:D:193:ASN:HB2	1:D:210:VAL:HG11	2.01	0.43
1:G:116:PHE:CD2	1:G:304:VAL:HG11	2.54	0.43
1:B:244:LEU:HD22	1:B:256:PHE:CD1	2.53	0.43
1:B:285:GLU:CD	1:B:285:GLU:N	2.72	0.43
1:D:4:THR:HG23	1:D:307:ALA:HB1	2.00	0.43
1:D:77:PHE:CD2	1:D:77:PHE:C	2.91	0.43
1:B:250:LEU:CD1	1:C:250:LEU:HD13	2.48	0.43
1:D:139:ILE:HA	1:D:143:LYS:O	2.18	0.43
1:D:244:LEU:CD2	1:D:256:PHE:CD1	2.95	0.43
1:G:116:PHE:CD2	1:G:304:VAL:CG1	3.02	0.43
1:A:104:ASN:OD1	1:A:106:ALA:HB3	2.18	0.43
1:A:207:ASP:OD1	1:A:209:SER:OG	2.27	0.43
1:B:118:ALA:HB3	1:B:257:ILE:HD13	2.01	0.43
1:B:222:ALA:HB1	1:B:268:LEU:HD21	2.01	0.43
1:B:144:LEU:HD23	1:B:146:ARG:CZ	2.49	0.43
1:F:167:CYS:HB3	1:F:171:SER:O	2.19	0.43
1:G:197:GLU:HG2	1:G:198:ASN:N	2.34	0.43
1:G:210:VAL:HG12	1:G:210:VAL:O	2.19	0.43
1:E:73:ALA:HA	1:E:89:LYS:HB2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:144:LEU:HD23	1:E:146:ARG:HH21	1.82	0.43
1:F:84:ARG:O	1:F:85:HIS:C	2.56	0.43
1:H:160:VAL:HG23	1:H:161:VAL:HG23	2.01	0.43
1:D:125:VAL:O	1:D:126:ILE:HD12	2.19	0.43
1:F:9:ILE:HD11	1:F:44:ILE:HD11	2.01	0.43
1:G:223:ARG:NH2	1:G:265:GLU:OE2	2.52	0.43
1:D:24:ARG:HB3	1:D:24:ARG:HH21	1.84	0.42
1:E:84:ARG:HA	1:E:85:HIS:HA	1.88	0.42
1:A:128:ILE:HD12	1:A:128:ILE:N	2.33	0.42
1:H:303:LEU:O	1:H:306:ALA:HB3	2.19	0.42
1:B:138:ILE:HG13	1:B:153:ALA:HB2	2.01	0.42
1:C:125:VAL:O	1:C:125:VAL:HG12	2.18	0.42
1:H:157:HIS:CE1	1:H:169:CYS:HB3	2.55	0.42
1:C:79:PRO:C	1:C:80:ASN:HD22	2.23	0.42
1:G:159:ARG:HD2	1:G:162:PRO:HA	2.00	0.42
1:H:307:ALA:O	1:H:310:ALA:HB3	2.20	0.42
1:C:178:TYR:HB3	1:C:239:TRP:CG	2.54	0.42
1:G:9:ILE:HD11	1:G:62:ILE:HG21	2.01	0.42
1:D:123:ASP:HA	1:D:142:ASN:HD21	1.85	0.42
1:D:134:LEU:H	1:D:176:GLU:HG2	1.85	0.42
1:F:3:LEU:HD22	1:F:3:LEU:HA	1.91	0.42
1:G:138:ILE:C	1:G:139:ILE:HD12	2.39	0.42
1:H:189:LYS:HZ3	1:H:211:ASP:HA	1.84	0.42
1:B:67:TYR:HB3	1:B:151:VAL:HG11	2.02	0.42
1:C:11:GLY:O	1:C:33:THR:HB	2.19	0.42
1:E:244:LEU:HD22	1:E:256:PHE:CD1	2.54	0.42
1:F:4:THR:HG23	1:F:307:ALA:HB1	2.01	0.42
1:H:3:LEU:HD12	1:H:57:VAL:HA	2.00	0.42
1:A:126:ILE:N	1:A:126:ILE:CD1	2.82	0.42
1:A:165:LEU:HD11	1:A:186:ARG:CZ	2.50	0.42
1:C:14:ILE:HD12	1:C:43:ALA:HB3	2.02	0.42
1:E:16:ALA:HB3	1:E:47:ALA:HB1	2.02	0.42
1:E:242:ALA:O	1:E:245:ALA:HB3	2.19	0.42
1:A:158:ILE:HG21	1:G:250:LEU:HD21	2.02	0.42
1:A:186:ARG:HE	1:D:172:GLN:HE22	1.67	0.42
1:B:188:ALA:O	1:B:189:LYS:C	2.58	0.42
1:B:164:GLY:O	1:B:172:GLN:HB3	2.20	0.42
1:B:165:LEU:HA	1:H:165:LEU:HD23	2.01	0.42
1:F:152:ALA:O	1:F:153:ALA:CB	2.66	0.42
1:H:126:ILE:HD11	1:H:251:PHE:CD1	2.55	0.42
1:H:177:GLN:HE22	1:H:182:ARG:HD2	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:175:TRP:CZ2	1:G:243:GLY:HA3	2.55	0.41
1:B:184:LEU:HB2	1:B:236:LEU:HD12	2.02	0.41
1:B:193:ASN:HD22	1:B:210:VAL:HG11	1.84	0.41
1:E:101:VAL:HG21	1:E:310:ALA:HA	2.01	0.41
1:H:73:ALA:CB	1:H:89:LYS:HG2	2.50	0.41
1:H:236:LEU:O	1:H:236:LEU:HD23	2.20	0.41
1:B:19:VAL:HA	1:B:24:ARG:O	2.20	0.41
1:C:41:VAL:HG12	1:C:41:VAL:O	2.20	0.41
1:D:219:SER:HB2	1:D:265:GLU:CD	2.41	0.41
1:E:270:LEU:HD13	1:E:294:ALA:HB2	2.01	0.41
1:F:4:THR:HG21	1:F:307:ALA:O	2.20	0.41
1:G:126:ILE:HG22	1:G:128:ILE:CD1	2.50	0.41
1:H:62:ILE:CD1	1:H:88:LEU:HD11	2.50	0.41
1:A:96:VAL:HG23	1:A:98:LEU:H	1.86	0.41
1:D:38:GLU:HA	1:D:41:VAL:HG23	2.02	0.41
1:D:83:TRP:O	1:D:84:ARG:HD2	2.21	0.41
1:E:10:GLY:N	1:E:13:LYS:O	2.53	0.41
1:A:149:PHE:CD2	1:G:288:PRO:HB2	2.56	0.41
1:B:12:THR:HG23	1:B:13:LYS:HG2	2.02	0.41
1:F:116:PHE:HB2	1:F:297:LEU:HD11	2.02	0.41
1:F:164:GLY:O	1:G:165:LEU:CD2	2.68	0.41
1:G:5:ILE:HG13	1:G:57:VAL:HG11	2.02	0.41
1:H:189:LYS:NZ	1:H:211:ASP:HA	2.35	0.41
1:H:271:ASP:HA	1:H:274:ARG:NH1	2.36	0.41
1:A:207:ASP:OD1	1:A:212:GLY:HA3	2.20	0.41
1:A:250:LEU:CD1	1:G:250:LEU:HD13	2.47	0.41
1:F:127:CYS:C	1:F:128:ILE:HD12	2.40	0.41
1:H:271:ASP:HB3	1:H:272:PRO:CD	2.51	0.41
1:B:73:ALA:HA	1:B:89:LYS:HB2	2.02	0.41
1:E:36:THR:HB	1:E:39:GLY:H	1.85	0.41
1:F:172:GLN:HE22	1:G:186:ARG:HE	1.69	0.41
1:H:183:ALA:O	1:H:184:LEU:C	2.59	0.41
1:B:283:GLY:O	1:B:287:ARG:CG	2.65	0.41
1:D:183:ALA:O	1:D:185:VAL:N	2.54	0.41
1:E:126:ILE:HD13	1:E:253:PRO:HB3	2.03	0.41
1:F:12:THR:HG23	1:F:13:LYS:HG2	2.02	0.41
1:C:111:TRP:CD2	1:C:309:LEU:HD21	2.55	0.40
1:D:73:ALA:HA	1:D:89:LYS:HB2	2.02	0.40
1:D:81:ILE:HG21	1:D:83:TRP:CE2	2.57	0.40
1:E:74:THR:CG2	1:E:85:HIS:HB3	2.52	0.40
1:D:3:LEU:C	1:D:3:LEU:HD13	2.41	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:101:VAL:CG2	1:E:310:ALA:HA	2.52	0.40
1:H:20:ASP:OD1	1:H:24:ARG:N	2.50	0.40
1:B:134:LEU:HD12	1:B:179:ALA:O	2.21	0.40
1:C:179:ALA:O	1:C:180:SER:HB3	2.20	0.40
1:E:7:VAL:HG13	1:E:16:ALA:HB2	2.02	0.40
1:G:10:GLY:O	1:G:12:THR:N	2.54	0.40
1:G:83:TRP:CD1	1:G:86:GLU:HB3	2.55	0.40
1:H:274:ARG:HG3	1:H:292:VAL:HB	2.02	0.40
1:B:164:GLY:HA3	1:B:178:TYR:OH	2.21	0.40
1:E:132:THR:HG22	1:E:182:ARG:NH2	2.36	0.40
1:G:309:LEU:HA	1:G:309:LEU:HD23	1.82	0.40
1:H:10:GLY:O	1:H:12:THR:N	2.55	0.40
1:D:220:GLU:O	1:D:222:ALA:N	2.55	0.40
1:D:281:LEU:HD12	1:D:282:ILE:N	2.37	0.40
1:G:95:ARG:HE	1:G:95:ARG:HB3	1.70	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	309/321 (96%)	286 (93%)	23 (7%)	0	100	100
1	B	310/321 (97%)	287 (93%)	20 (6%)	3 (1%)	15	47
1	C	308/321 (96%)	279 (91%)	26 (8%)	3 (1%)	15	47
1	D	309/321 (96%)	281 (91%)	28 (9%)	0	100	100
1	E	308/321 (96%)	284 (92%)	23 (8%)	1 (0%)	41	72
1	F	308/321 (96%)	287 (93%)	20 (6%)	1 (0%)	41	72
1	G	309/321 (96%)	282 (91%)	24 (8%)	3 (1%)	15	47
1	H	308/321 (96%)	272 (88%)	34 (11%)	2 (1%)	25	59

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	2469/2568 (96%)	2258 (92%)	198 (8%)	13 (0%)	29 62

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	238	ARG
1	C	180	SER
1	H	11	GLY
1	B	156	GLY
1	B	301	ALA
1	C	11	GLY
1	G	11	GLY
1	G	142	ASN
1	G	264	ASP
1	H	88	LEU
1	E	81	ILE
1	C	35	PRO
1	F	298	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	218/227 (96%)	196 (90%)	22 (10%)	7 27
1	B	218/227 (96%)	204 (94%)	14 (6%)	17 47
1	C	218/227 (96%)	196 (90%)	22 (10%)	7 27
1	D	218/227 (96%)	199 (91%)	19 (9%)	10 34
1	E	218/227 (96%)	198 (91%)	20 (9%)	9 31
1	F	218/227 (96%)	199 (91%)	19 (9%)	10 34
1	G	218/227 (96%)	198 (91%)	20 (9%)	9 31
1	H	218/227 (96%)	191 (88%)	27 (12%)	4 19
All	All	1744/1816 (96%)	1581 (91%)	163 (9%)	9 30

All (163) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	LEU
1	A	12	THR
1	A	22	GLU
1	A	35	PRO
1	A	36	THR
1	A	71	LYS
1	A	79	PRO
1	A	115	ARG
1	A	126	ILE
1	A	143	LYS
1	A	158	ILE
1	A	166	LEU
1	A	195	THR
1	A	213	ILE
1	A	251	PHE
1	A	270	LEU
1	A	279	ARG
1	A	281	LEU
1	A	282	ILE
1	A	286	TRP
1	A	287	ARG
1	A	312	GLN
1	B	74	THR
1	B	115	ARG
1	B	120	GLN
1	B	129	THR
1	B	143	LYS
1	B	158	ILE
1	B	216	LYS
1	B	219	SER
1	B	278	ARG
1	B	279	ARG
1	B	280	TRP
1	B	285	GLU
1	B	287	ARG
1	B	312	GLN
1	C	3	LEU
1	C	13	LYS
1	C	36	THR
1	C	56	ASP
1	C	80	ASN
1	C	96	VAL

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Mol	Chain	Res	Type
1	C	130	LEU
1	C	143	LYS
1	C	158	ILE
1	C	171	SER
1	C	195	THR
1	C	205	LEU
1	C	219	SER
1	C	234	ARG
1	C	254	SER
1	C	263	SER
1	C	265	GLU
1	C	270	LEU
1	C	280	TRP
1	C	287	ARG
1	C	296	GLN
1	C	297	LEU
1	D	12	THR
1	D	24	ARG
1	D	27	SER
1	D	36	THR
1	D	101	VAL
1	D	115	ARG
1	D	143	LYS
1	D	151	VAL
1	D	166	LEU
1	D	171	SER
1	D	195	THR
1	D	219	SER
1	D	262	VAL
1	D	270	LEU
1	D	279	ARG
1	D	280	TRP
1	D	282	ILE
1	D	287	ARG
1	D	312	GLN
1	E	3	LEU
1	E	4	THR
1	E	31	VAL
1	E	36	THR
1	E	38	GLU
1	E	56	ASP
1	E	74	THR

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Mol	Chain	Res	Type
1	E	84	ARG
1	E	124	ASP
1	E	143	LYS
1	E	171	SER
1	E	190	GLN
1	E	205	LEU
1	E	211	ASP
1	E	214	GLU
1	E	219	SER
1	E	234	ARG
1	E	264	ASP
1	E	279	ARG
1	E	287	ARG
1	F	3	LEU
1	F	13	LYS
1	F	21	GLU
1	F	36	THR
1	F	38	GLU
1	F	101	VAL
1	F	115	ARG
1	F	124	ASP
1	F	129	THR
1	F	158	ILE
1	F	209	SER
1	F	210	VAL
1	F	254	SER
1	F	279	ARG
1	F	282	ILE
1	F	285	GLU
1	F	287	ARG
1	F	296	GLN
1	F	312	GLN
1	G	3	LEU
1	G	12	THR
1	G	36	THR
1	G	70	ASP
1	G	71	LYS
1	G	74	THR
1	G	80	ASN
1	G	81	ILE
1	G	82	ASP
1	G	101	VAL

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Mol	Chain	Res	Type
1	G	115	ARG
1	G	123	ASP
1	G	158	ILE
1	G	182	ARG
1	G	209	SER
1	G	231	ASP
1	G	263	SER
1	G	270	LEU
1	G	280	TRP
1	G	287	ARG
1	H	25	ILE
1	H	27	SER
1	H	28	THR
1	H	36	THR
1	H	38	GLU
1	H	42	ASP
1	H	45	CYS
1	H	56	ASP
1	H	76	LEU
1	H	88	LEU
1	H	89	LYS
1	H	90	ASP
1	H	98	LEU
1	H	115	ARG
1	H	116	PHE
1	H	120	GLN
1	H	142	ASN
1	H	144	LEU
1	H	158	ILE
1	H	182	ARG
1	H	228	VAL
1	H	278	ARG
1	H	282	ILE
1	H	285	GLU
1	H	287	ARG
1	H	289	HIS
1	H	312	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	142	ASN

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Mol	Chain	Res	Type
1	A	172	GLN
1	A	193	ASN
1	A	198	ASN
1	A	217	HIS
1	A	312	GLN
1	B	80	ASN
1	B	172	GLN
1	B	190	GLN
1	B	193	ASN
1	B	312	GLN
1	C	80	ASN
1	C	172	GLN
1	C	193	ASN
1	C	198	ASN
1	C	224	GLN
1	C	289	HIS
1	D	142	ASN
1	D	172	GLN
1	D	190	GLN
1	D	193	ASN
1	D	217	HIS
1	D	296	GLN
1	E	224	GLN
1	E	312	GLN
1	F	80	ASN
1	F	172	GLN
1	F	190	GLN
1	F	193	ASN
1	F	198	ASN
1	F	312	GLN
1	G	80	ASN
1	G	120	GLN
1	G	190	GLN
1	G	193	ASN
1	G	198	ASN
1	G	296	GLN
1	H	80	ASN
1	H	122	HIS
1	H	177	GLN
1	H	193	ASN
1	H	198	ASN
1	H	289	HIS

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 monosaccharides in this entry.

5.6 Ligand geometry

Of 10 ligands modelled in this entry, 8 are 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	SO4	B	323	-	4,4,4	0.22	0	6,6,6	0.22	0
3	SO4	E	323	-	4,4,4	0.12	0	6,6,6	0.33	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

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	311/321 (96%)	-0.42	1 (0%) 94 94	60, 81, 106, 116	0
1	B	312/321 (97%)	-0.38	2 (0%) 89 89	60, 84, 111, 122	0
1	C	310/321 (96%)	-0.37	0 100 100	58, 84, 111, 119	0
1	D	311/321 (96%)	-0.30	1 (0%) 94 94	58, 82, 107, 117	0
1	E	310/321 (96%)	-0.37	2 (0%) 89 89	60, 82, 113, 125	0
1	F	310/321 (96%)	-0.42	1 (0%) 94 94	62, 83, 112, 120	0
1	G	311/321 (96%)	-0.36	1 (0%) 94 94	60, 84, 111, 120	0
1	H	310/321 (96%)	-0.21	8 (2%) 56 52	57, 99, 160, 171	0
All	All	2485/2568 (96%)	-0.35	16 (0%) 89 89	57, 84, 116, 171	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	6	GLY	4.0
1	H	94	GLN	3.9
1	B	2	GLY	3.5
1	H	12	THR	3.1
1	E	80	ASN	2.6
1	H	17	GLY	2.6
1	H	56	ASP	2.6
1	H	54	GLY	2.3
1	H	55	HIS	2.2
1	F	12	THR	2.2
1	G	123	ASP	2.2
1	E	61	GLY	2.1
1	A	120	GLN	2.0
1	D	132	THR	2.0
1	B	12	THR	2.0
1	H	120	GLN	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 monosaccharides 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. 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
3	SO4	E	323	5/5	0.89	0.18	110,110,111,112	0
3	SO4	B	323	5/5	0.90	0.20	114,115,115,115	0
2	ZN	G	322	1/1	0.99	0.05	75,75,75,75	0
2	ZN	H	322	1/1	0.99	0.04	79,79,79,79	0
2	ZN	D	322	1/1	0.99	0.04	79,79,79,79	0
2	ZN	F	322	1/1	0.99	0.04	70,70,70,70	0
2	ZN	C	322	1/1	1.00	0.04	81,81,81,81	0
2	ZN	A	322	1/1	1.00	0.04	82,82,82,82	0
2	ZN	E	322	1/1	1.00	0.05	73,73,73,73	0
2	ZN	B	322	1/1	1.00	0.04	77,77,77,77	0

6.5 Other polymers (i)

There are no such residues in this entry.