Full wwPDB X-ray Structure Validation Report

Feb 1, 2016 – 05:28 AM GMT

PDB ID	:	2QTS
Title	:	Structure of an acid-sensing ion channel 1 at 1.9 A resolution and low pH
Authors	:	Jasti, J.; Furukawa, H.; Gonzales, E.B.; Gouaux, E.
Deposited on	:	2007-08-02
Resolution	:	1.90 Å(reported)

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

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

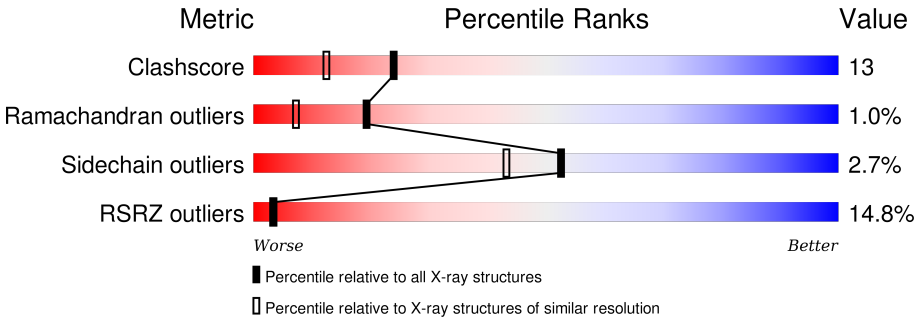
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 1.90 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))
Clashscore	102246	5398 (1.90-1.90)
Ramachandran outliers	100387	5338 (1.90-1.90)
Sidechain outliers	100360	5339 (1.90-1.90)
RSRZ outliers	91569	4766 (1.90-1.90)

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	438	13% 69% 23% • 5%
1	B	438	12% 73% 21% • •
1	C	438	10% 71% 22% • 5%
1	D	438	18% 69% 24% • 5%
1	E	438	16% 70% 25% • •
1	F	438	16% 71% 20% • 6%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	MAL	C	3	-	-	-	X
3	NAG	A	1	-	-	-	X
3	NAG	F	11	-	-	-	X

2 Entry composition

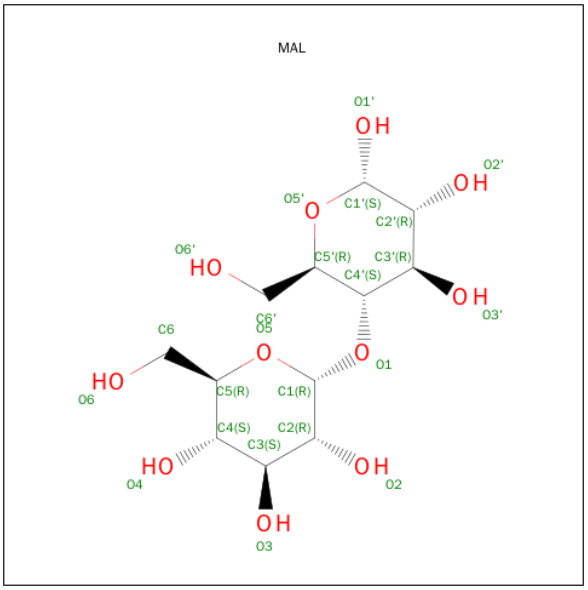
There are 5 unique types of molecules in this entry. The entry contains 22034 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Acid-sensing ion channel.

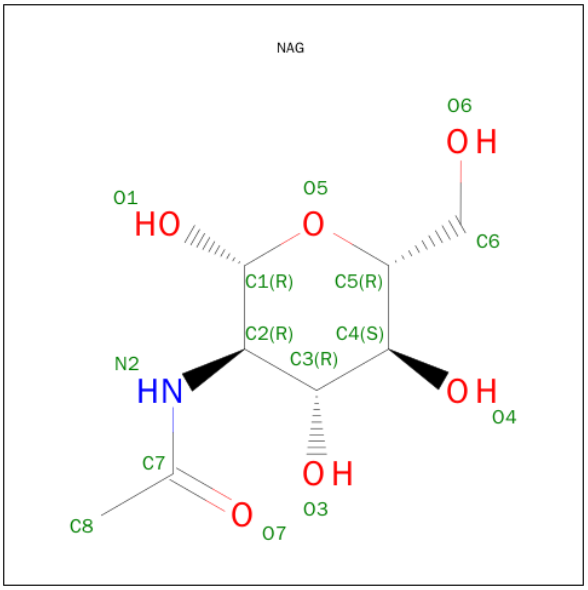
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	417	Total	C	N	O	S	0	0	0
			3345	2144	541	633	27			
1	B	420	Total	C	N	O	S	0	0	0
			3369	2161	545	636	27			
1	C	418	Total	C	N	O	S	0	0	0
			3350	2148	542	633	27			
1	D	415	Total	C	N	O	S	0	0	0
			3324	2130	539	628	27			
1	E	421	Total	C	N	O	S	0	0	0
			3375	2164	546	638	27			
1	F	412	Total	C	N	O	S	0	0	0
			3299	2114	536	622	27			

- Molecule 2 is SUGAR (MALTOSE) (three-letter code: MAL) (formula: $C_{12}H_{22}O_{11}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total C O 23 12 11	0	0
2	B	1	Total C O 23 12 11	0	0
2	C	1	Total C O 23 12 11	0	0

- Molecule 3 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O 14 8 1 5	0	0
3	A	1	Total C N O 14 8 1 5	0	0
3	B	1	Total C N O 14 8 1 5	0	0
3	B	1	Total C N O 14 8 1 5	0	0
3	C	1	Total C N O 14 8 1 5	0	0
3	C	1	Total C N O 14 8 1 5	0	0
3	D	1	Total C N O 14 8 1 5	0	0
3	D	1	Total C N O 14 8 1 5	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	E	1	Total C N O 14 8 1 5	0	0
3	E	1	Total C N O 14 8 1 5	0	0
3	F	1	Total C N O 14 8 1 5	0	0
3	F	1	Total C N O 14 8 1 5	0	0

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	D	1	Total Cl 1 1	0	0
4	E	1	Total Cl 1 1	0	0
4	B	1	Total Cl 1 1	0	0
4	C	1	Total Cl 1 1	0	0
4	A	1	Total Cl 1 1	0	0
4	F	1	Total Cl 1 1	0	0

- Molecule 5 is water.

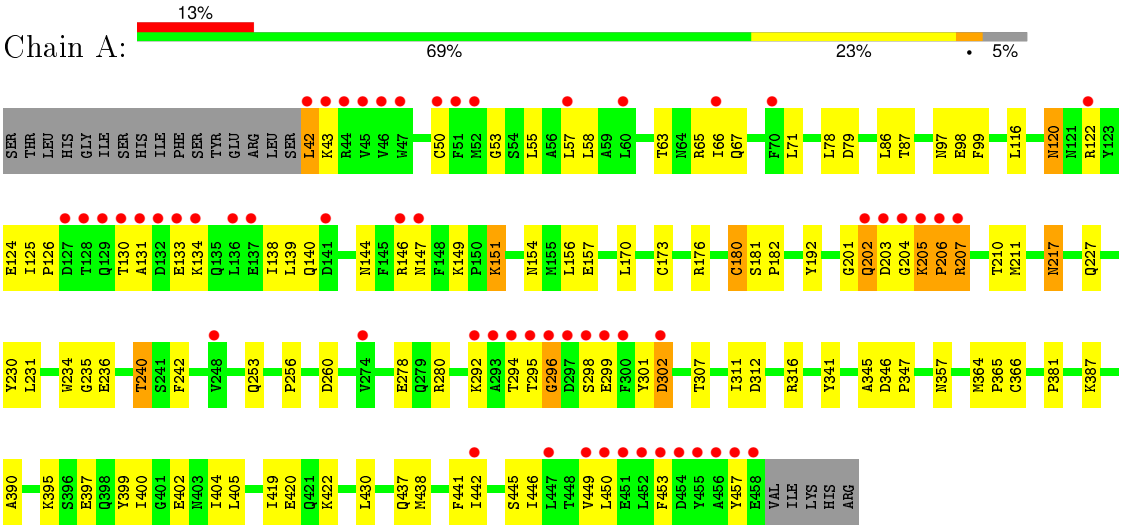
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	285	Total O 285 285	0	0
5	B	280	Total O 280 280	0	0
5	C	302	Total O 302 302	0	0
5	D	270	Total O 270 270	0	0
5	E	292	Total O 292 292	0	0
5	F	300	Total O 300 300	0	0

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.

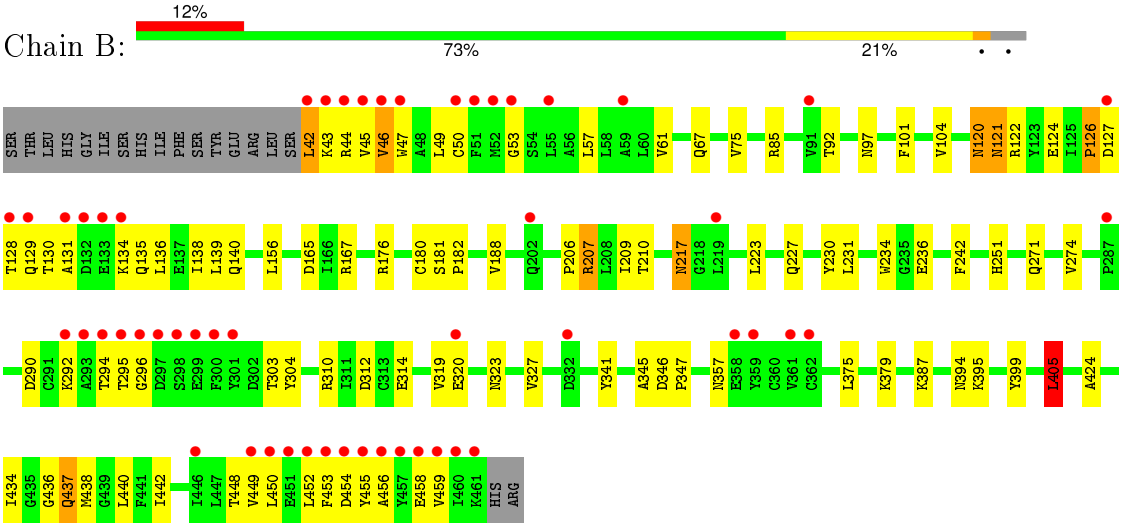
- Molecule 1: Acid-sensing ion channel

Chain A:



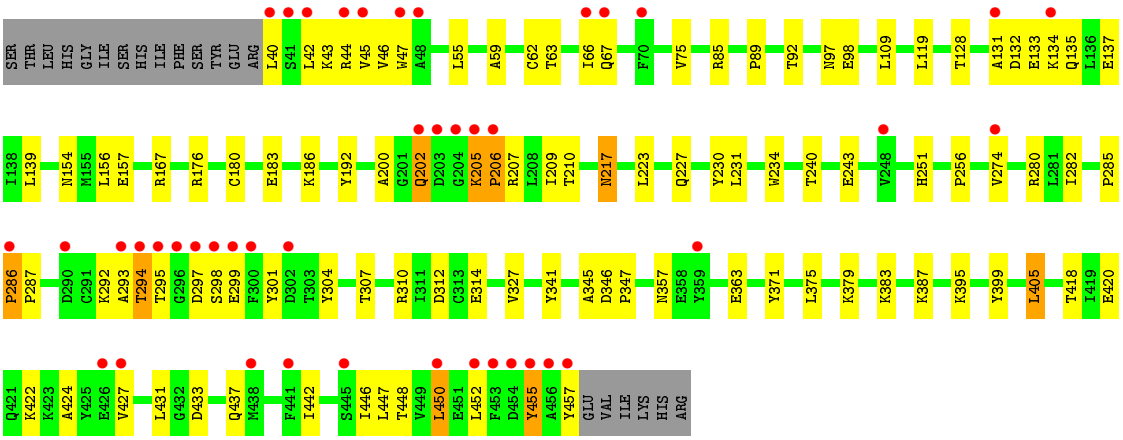
- Molecule 1: Acid-sensing ion channel

Chain B:



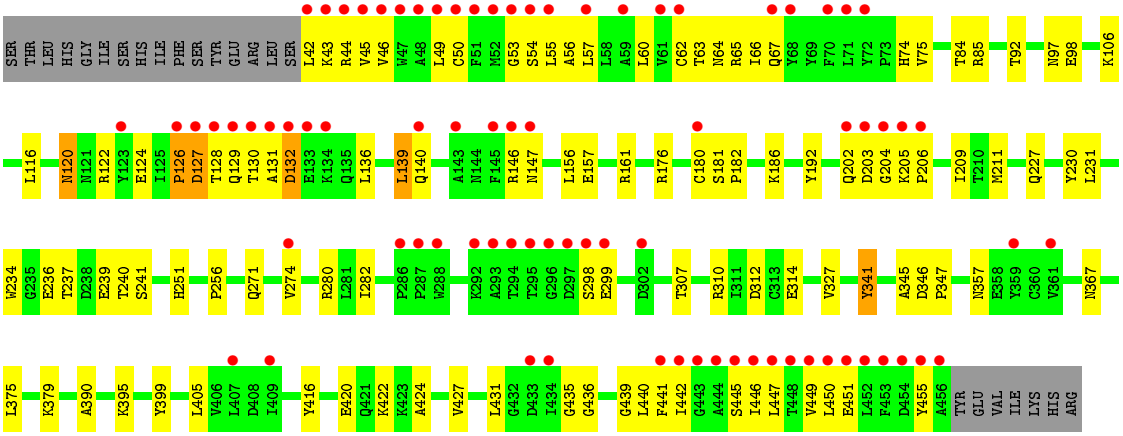
- Molecule 1: Acid-sensing ion channel

Chain C:



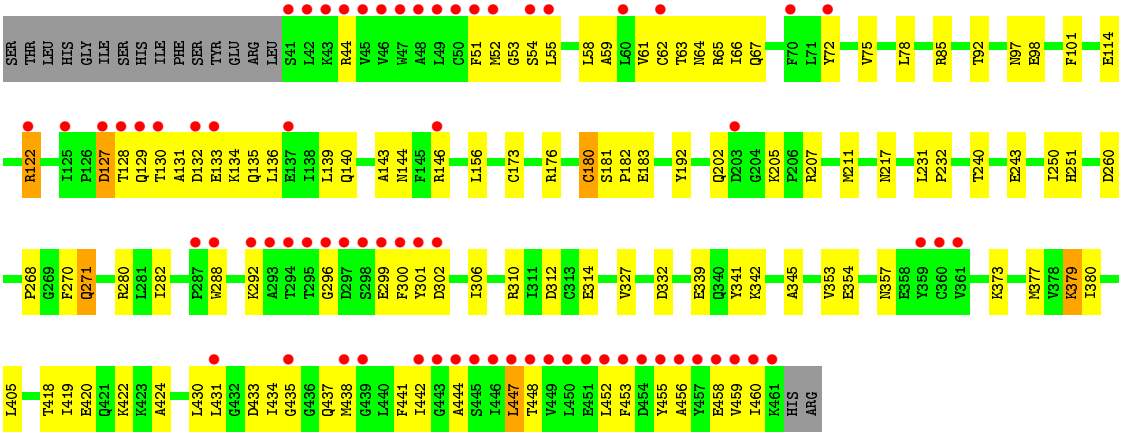
• Molecule 1: Acid-sensing ion channel

Chain D:



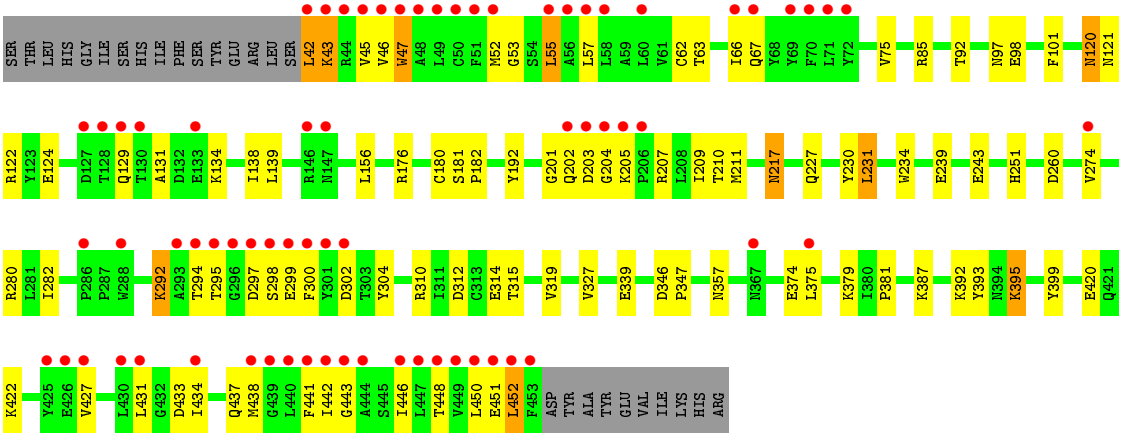
• Molecule 1: Acid-sensing ion channel

Chain E:



• Molecule 1: Acid-sensing ion channel

Chain F:


SER THR LEU HIS GLY ILE SER HIS ILE PHE SER TYR GLU ARG LEU SER L42 K43 R44 V45 V46 W47 A48 L49 C50 F51 M52 G53 S54 L55 A56 L57 L58 A59 L60 V61 C62 T63 I66 Q67 Y68 Y69 F70 L71 Y72 V75 R85 T92 N97 E98 F101 N120 N121
R122 Y123 E124 D127 T128 Q129 T130 A131 D132 E133 K134 I138 L139 R146 N147 L156 R176 C180 S181 P182 Y192 G201 Q202 D203 G204 K205 P206 R207 L208 I209 T210 M211 N217 Q227 Y230 L231 W234 E239 E243 H251 D260 V274
R280 L281 I282 P286 P287 W288 K292 A293 T294 T295 G296 D297 S298 E299 F300 Y301 D302 T303 Y304 R310 I311 D312 C313 E314 T315 V319 V327 E339 D346 P347 N357 N367 E374 L375 K379 I380 P381 K387 K392 Y393 N394 K395 Y399 E420 Q421
K422 Y425 E426 V427 L430 L431 G432 D433 I434 Q437 M438 G439 L440 F441 I442 G443 A444 S445 I446 L447 T448 V449 L450 E451 L452 F453 ASP TYR ALA TYR GLU VAL ILE LYS HIS ARG

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	124.25Å 110.78Å 149.89Å 90.00° 97.54° 90.00°	Depositor
Resolution (Å)	30.00 – 1.90 49.53 – 1.76	Depositor EDS
% Data completeness (in resolution range)	88.4 (30.00-1.90) 77.2 (49.53-1.76)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	1.48 (at 1.76Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.208 , 0.233 0.214 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å^2)	20.2	Xtriage
Anisotropy	0.472	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 56.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 327387 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	22034	wwPDB-VP
Average B, all atoms (Å^2)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.21% 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: CL, MAL, NAG

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	0.32	0/3424	0.58	0/4637
1	B	0.32	0/3448	0.59	1/4669 (0.0%)
1	C	0.33	0/3429	0.60	0/4644
1	D	0.32	0/3402	0.58	0/4607
1	E	0.32	0/3454	0.59	1/4677 (0.0%)
1	F	0.32	0/3376	0.59	0/4571
All	All	0.32	0/20533	0.59	2/27805 (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	405	LEU	CA-CB-CG	6.13	129.40	115.30
1	E	271	GLN	N-CA-C	-5.00	97.49	111.00

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	3345	0	3238	91	0
1	B	3369	0	3271	103	0
1	C	3350	0	3248	95	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	3324	0	3222	99	0
1	E	3375	0	3276	100	0
1	F	3299	0	3205	82	0
2	B	46	0	44	0	0
2	C	23	0	22	0	0
3	A	28	0	26	0	0
3	B	28	0	26	0	0
3	C	28	0	26	1	0
3	D	28	0	26	1	0
3	E	28	0	26	0	0
3	F	28	0	26	1	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
5	A	285	0	0	9	0
5	B	280	0	0	3	0
5	C	302	0	0	9	0
5	D	270	0	0	9	0
5	E	292	0	0	7	0
5	F	300	0	0	7	0
All	All	22034	0	19682	523	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 (523) 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:D:131:ALA:HA	1:F:387:LYS:HD3	1.46	0.98
1:F:294:THR:HG23	1:F:304:TYR:H	1.28	0.97
1:F:298:SER:HB2	1:F:302:ASP:HA	1.47	0.95
1:B:131:ALA:HB2	1:B:234:TRP:HE1	1.31	0.93
1:C:294:THR:HA	1:C:304:TYR:HB3	1.50	0.91
1:B:42:LEU:HD12	1:B:44:ARG:HB2	1.54	0.88
1:B:207:ARG:HH21	1:B:207:ARG:HB2	1.41	0.85
1:E:122:ARG:HE	1:E:122:ARG:HA	1.41	0.83
1:A:154:ASN:HD22	1:A:157:GLU:H	1.27	0.82
1:C:186:LYS:HE2	1:C:202:GLN:HG2	1.60	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:205:LYS:HB3	1:D:206:PRO:HD2	1.63	0.80
1:D:211:MET:HG3	1:E:357:ASN:ND2	1.98	0.79
1:D:98:GLU:HG2	1:D:192:TYR:O	1.84	0.78
1:D:357:ASN:ND2	1:F:211:MET:HG3	1.98	0.77
1:C:223:LEU:HB2	1:C:405:LEU:CD2	2.14	0.77
1:E:146:ARG:HD2	5:E:671:HOH:O	1.83	0.76
1:A:395:LYS:HG2	1:A:399:TYR:CD1	2.19	0.76
1:E:127:ASP:CG	1:E:128:THR:H	1.90	0.74
1:C:42:LEU:H	1:C:42:LEU:HD22	1.52	0.74
1:D:127:ASP:O	1:D:130:THR:HG23	1.87	0.73
1:C:395:LYS:HG2	1:C:399:TYR:CD1	2.24	0.73
1:B:97:ASN:HD21	1:B:231:LEU:H	1.36	0.73
1:A:130:THR:HB	1:C:387:LYS:HB3	1.70	0.72
1:F:98:GLU:HG2	1:F:192:TYR:O	1.88	0.72
1:C:223:LEU:HB2	1:C:405:LEU:HD21	1.72	0.71
1:E:65:ARG:HH21	1:E:433:ASP:HB3	1.56	0.71
1:E:420:GLU:HG2	1:E:422:LYS:HD3	1.71	0.71
1:A:78:LEU:HD13	1:A:79:ASP:N	2.05	0.70
1:A:176:ARG:HH22	1:B:357:ASN:ND2	1.89	0.70
1:C:98:GLU:HG2	1:C:192:TYR:O	1.91	0.70
1:D:395:LYS:HG2	1:D:399:TYR:CD1	2.27	0.70
1:F:310:ARG:O	1:F:314:GLU:HG3	1.92	0.69
1:D:63:THR:O	1:D:67:GLN:HG3	1.92	0.69
1:D:156:LEU:HD13	1:D:327:VAL:HG13	1.72	0.69
1:E:63:THR:O	1:E:67:GLN:HG3	1.92	0.69
1:B:437:GLN:NE2	1:B:437:GLN:H	1.90	0.69
1:E:144:ASN:OD1	1:E:146:ARG:HD3	1.93	0.69
1:C:405:LEU:HD23	1:C:405:LEU:O	1.94	0.67
1:C:210:THR:HG23	1:C:217:ASN:HB3	1.75	0.67
1:D:239:GLU:HB2	5:D:705:HOH:O	1.94	0.67
1:E:296:GLY:HA2	1:E:302:ASP:HA	1.77	0.67
1:A:357:ASN:HD21	1:C:176:ARG:HH12	1.43	0.66
1:E:332:ASP:HB3	5:E:700:HOH:O	1.96	0.66
1:B:341:TYR:HA	1:B:345:ALA:HB3	1.78	0.65
1:B:120:ASN:ND2	1:B:122:ARG:H	1.94	0.65
1:C:240:THR:HG21	5:C:726:HOH:O	1.97	0.65
1:F:42:LEU:HD13	1:F:42:LEU:N	2.11	0.65
1:B:120:ASN:HD22	1:B:120:ASN:C	1.98	0.65
1:A:86:LEU:HD23	1:A:87:THR:N	2.12	0.65
1:A:366:CYS:HB2	5:A:692:HOH:O	1.97	0.64
1:D:375:LEU:HD13	5:F:591:HOH:O	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:97:ASN:HD21	1:A:231:LEU:H	1.43	0.64
1:D:131:ALA:HB3	1:D:234:TRP:HE1	1.61	0.64
1:F:393:TYR:O	1:F:395:LYS:HD2	1.97	0.64
1:B:450:LEU:HD21	1:C:42:LEU:HB2	1.78	0.64
1:A:260:ASP:HB3	5:A:732:HOH:O	1.98	0.64
1:D:310:ARG:O	1:D:314:GLU:HG3	1.97	0.64
1:D:341:TYR:HA	1:D:345:ALA:HB3	1.80	0.64
1:E:122:ARG:HA	1:E:122:ARG:NE	2.11	0.64
1:D:203:ASP:HB3	1:D:205:LYS:HG3	1.80	0.64
1:F:298:SER:CB	1:F:302:ASP:HA	2.25	0.64
1:B:437:GLN:H	1:B:437:GLN:HE21	1.45	0.63
1:A:387:LYS:HD3	5:A:733:HOH:O	1.97	0.63
1:A:139:LEU:HD23	1:A:234:TRP:CH2	2.33	0.63
1:A:78:LEU:HD23	1:A:419:ILE:HG12	1.80	0.63
1:C:75:VAL:HG13	1:C:424:ALA:HB2	1.79	0.63
1:D:176:ARG:HH22	1:E:357:ASN:ND2	1.95	0.63
1:A:420:GLU:OE1	1:A:422:LYS:HE2	1.98	0.63
1:B:156:LEU:HD13	1:B:327:VAL:HG13	1.79	0.63
1:F:97:ASN:HD21	1:F:231:LEU:H	1.46	0.62
1:A:67:GLN:O	1:A:71:LEU:HD23	2.00	0.62
1:E:55:LEU:HD13	1:E:55:LEU:O	1.98	0.62
1:F:55:LEU:HD23	1:F:441:PHE:CE1	2.35	0.62
1:A:295:THR:HG22	1:A:296:GLY:N	2.14	0.62
1:B:176:ARG:HH12	1:C:357:ASN:HD21	1.45	0.62
1:B:379:LYS:HE3	5:B:496:HOH:O	1.98	0.62
1:F:239:GLU:HB2	5:F:640:HOH:O	1.98	0.62
1:C:156:LEU:HD13	1:C:327:VAL:HG13	1.81	0.61
1:C:132:ASP:HB3	1:C:135:GLN:HG3	1.82	0.61
1:A:125:ILE:HD12	1:A:140:GLN:HG2	1.80	0.61
1:B:45:VAL:C	1:B:47:TRP:H	2.04	0.61
1:E:211:MET:HG3	1:F:357:ASN:ND2	2.16	0.61
1:B:295:THR:HG22	1:B:296:GLY:N	2.16	0.61
1:C:285:PRO:CB	1:C:286:PRO:HD2	2.30	0.61
1:C:418:THR:HG23	5:C:532:HOH:O	2.01	0.61
1:E:310:ARG:O	1:E:314:GLU:HG3	2.00	0.60
1:B:395:LYS:HG2	1:B:399:TYR:CD1	2.36	0.60
1:E:59:ALA:HB2	1:E:441:PHE:CE2	2.36	0.60
1:D:75:VAL:HG13	1:D:424:ALA:HB2	1.82	0.60
1:E:438:MET:O	1:E:442:ILE:HG13	2.00	0.60
1:C:40:LEU:HD22	1:C:43:LYS:HE3	1.83	0.60
1:F:62:CYS:O	1:F:66:ILE:HG13	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:97:ASN:HD21	1:D:231:LEU:H	1.50	0.60
1:F:120:ASN:ND2	1:F:122:ARG:H	2.00	0.60
1:E:456:ALA:O	1:E:460:ILE:HG13	2.02	0.59
1:E:341:TYR:HA	1:E:345:ALA:HB3	1.84	0.59
1:C:298:SER:HB2	1:C:301:TYR:O	2.02	0.59
1:C:200:ALA:HB1	1:C:202:GLN:NE2	2.17	0.59
1:D:62:CYS:O	1:D:66:ILE:HG12	2.02	0.59
1:B:92:THR:OG1	1:B:251:HIS:HE1	1.85	0.59
1:C:202:GLN:HE21	1:C:202:GLN:N	2.01	0.59
1:A:176:ARG:HH12	1:B:357:ASN:HD21	1.49	0.59
1:F:101:PHE:HE1	1:F:139:LEU:HD21	1.68	0.59
1:E:139:LEU:O	1:E:143:ALA:N	2.35	0.58
1:E:136:LEU:O	1:E:140:GLN:HG3	2.02	0.58
1:D:120:ASN:ND2	1:D:124:GLU:H	2.00	0.58
1:A:154:ASN:HD21	1:A:156:LEU:HB3	1.68	0.58
1:B:454:ASP:CG	1:C:40:LEU:HD21	2.24	0.58
1:C:47:TRP:HZ3	1:C:447:LEU:HB3	1.69	0.58
1:E:97:ASN:HD21	1:E:231:LEU:H	1.52	0.58
1:D:50:CYS:HB2	1:F:450:LEU:HD21	1.84	0.58
1:D:120:ASN:C	1:D:120:ASN:HD22	2.07	0.58
1:E:240:THR:HG21	5:E:623:HOH:O	2.02	0.58
1:E:260:ASP:HB3	5:E:583:HOH:O	2.03	0.58
1:C:63:THR:O	1:C:67:GLN:HG3	2.04	0.57
1:E:176:ARG:HH12	1:F:357:ASN:HD21	1.51	0.57
1:F:120:ASN:HD22	1:F:120:ASN:C	2.07	0.57
1:E:181:SER:OG	1:E:183:GLU:HG2	2.05	0.57
1:E:62:CYS:O	1:E:66:ILE:HG13	2.05	0.57
1:A:120:ASN:C	1:A:120:ASN:HD22	2.08	0.57
1:E:207:ARG:NH1	1:E:207:ARG:HB2	2.20	0.57
1:A:98:GLU:HG2	1:A:192:TYR:O	2.05	0.57
1:D:120:ASN:ND2	1:D:122:ARG:H	2.02	0.57
1:F:207:ARG:HA	5:F:551:HOH:O	2.03	0.57
1:B:437:GLN:N	1:B:437:GLN:NE2	2.53	0.57
1:B:120:ASN:HD22	1:B:122:ARG:H	1.52	0.57
1:E:53:GLY:C	1:E:55:LEU:H	2.08	0.57
1:A:253:GLN:HG3	5:A:578:HOH:O	2.05	0.57
1:D:43:LYS:NZ	1:D:43:LYS:HB3	2.20	0.57
1:B:223:LEU:HB2	1:B:405:LEU:HD22	1.87	0.57
1:C:341:TYR:HA	1:C:345:ALA:HB3	1.86	0.57
1:C:154:ASN:HD22	1:C:157:GLU:H	1.53	0.56
1:A:298:SER:HB3	1:A:302:ASP:HA	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:357:ASN:ND2	1:F:176:ARG:HH22	2.03	0.56
1:F:203:ASP:O	1:F:205:LYS:HG2	2.05	0.56
1:B:207:ARG:HB2	1:B:207:ARG:NH2	2.17	0.56
1:D:157:GLU:OE2	1:D:161:ARG:NE	2.34	0.56
1:C:285:PRO:HB2	1:C:286:PRO:HD2	1.86	0.56
1:B:75:VAL:HG23	1:B:424:ALA:HB2	1.86	0.56
1:C:167:ARG:NH2	1:C:183:GLU:OE1	2.39	0.56
1:D:53:GLY:O	1:D:57:LEU:HG	2.06	0.56
1:F:420:GLU:OE1	1:F:422:LYS:HE2	2.06	0.56
1:B:128:THR:HB	1:B:136:LEU:HD21	1.87	0.56
1:B:42:LEU:C	1:B:44:ARG:H	2.08	0.56
1:B:127:ASP:O	1:B:130:THR:HG23	2.06	0.56
1:D:442:ILE:HG22	1:E:54:SER:OG	2.05	0.56
1:B:295:THR:HG22	1:B:296:GLY:H	1.70	0.56
1:C:97:ASN:HD21	1:C:231:LEU:H	1.54	0.56
1:C:282:ILE:HB	1:C:420:GLU:HG3	1.88	0.56
1:F:92:THR:OG1	1:F:251:HIS:HE1	1.89	0.56
1:B:206:PRO:HG2	5:B:648:HOH:O	2.06	0.56
1:E:176:ARG:HH22	1:F:357:ASN:ND2	2.04	0.56
1:A:210:THR:HG22	1:A:217:ASN:O	2.06	0.55
1:F:53:GLY:O	1:F:57:LEU:HD23	2.06	0.55
1:F:156:LEU:HD13	1:F:327:VAL:HG13	1.87	0.55
1:B:405:LEU:C	1:B:405:LEU:HD23	2.27	0.55
1:A:42:LEU:HD13	1:A:42:LEU:N	2.21	0.55
1:A:65:ARG:NE	1:A:65:ARG:HA	2.22	0.55
1:A:50:CYS:HB3	1:C:446:ILE:HG23	1.89	0.55
1:D:447:LEU:HD12	1:F:450:LEU:HB3	1.88	0.55
1:A:204:GLY:O	1:A:205:LYS:C	2.45	0.55
1:F:131:ALA:HB2	1:F:234:TRP:HE1	1.72	0.55
1:E:420:GLU:CG	1:E:422:LYS:HD3	2.37	0.55
1:A:211:MET:HG3	1:B:357:ASN:ND2	2.21	0.55
1:C:133:GLU:CD	1:C:133:GLU:H	2.09	0.55
1:D:447:LEU:O	1:D:451:GLU:HG3	2.06	0.55
1:A:122:ARG:O	1:A:124:GLU:HG3	2.07	0.55
1:D:237:THR:OG1	1:D:240:THR:HG23	2.07	0.55
1:A:280:ARG:HG2	1:A:280:ARG:HH11	1.72	0.55
1:E:452:LEU:HD23	1:E:452:LEU:O	2.06	0.55
1:B:139:LEU:HD23	1:B:234:TRP:CH2	2.42	0.54
1:A:295:THR:HG22	1:A:296:GLY:H	1.71	0.54
1:F:134:LYS:O	1:F:138:ILE:HG12	2.06	0.54
1:D:357:ASN:HD21	1:F:176:ARG:HH12	1.54	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:357:ASN:HD22	1:F:211:MET:HG3	1.72	0.54
1:A:294:THR:HG22	1:A:295:THR:N	2.21	0.54
3:F:11:NAG:O3	3:F:11:NAG:H83	2.07	0.54
1:E:455:TYR:O	1:E:459:VAL:HG23	2.07	0.54
1:C:299:GLU:HG2	1:C:312:ASP:OD1	2.08	0.54
1:D:146:ARG:O	1:D:147:ASN:HB2	2.07	0.54
1:C:286:PRO:HG2	1:C:287:PRO:HD3	1.89	0.54
1:B:130:THR:HA	5:B:739:HOH:O	2.06	0.54
1:E:250:ILE:HD12	1:E:373:LYS:HD3	1.89	0.54
1:C:387:LYS:HD3	1:C:387:LYS:O	2.07	0.54
1:E:64:ASN:HA	1:E:67:GLN:NE2	2.23	0.54
1:F:121:ASN:OD1	1:F:122:ARG:HG3	2.06	0.54
1:D:240:THR:HG21	5:D:546:HOH:O	2.06	0.54
1:B:236:GLU:HG2	1:B:242:PHE:CZ	2.42	0.54
1:D:157:GLU:CD	1:D:161:ARG:HE	2.10	0.54
1:F:210:THR:HG23	1:F:217:ASN:HB3	1.90	0.54
1:C:59:ALA:O	1:C:63:THR:HG23	2.08	0.54
1:F:280:ARG:HG2	1:F:280:ARG:HH21	1.73	0.54
1:A:154:ASN:ND2	1:A:157:GLU:H	2.03	0.54
1:E:128:THR:HA	1:E:136:LEU:HD21	1.88	0.54
1:A:442:ILE:O	1:A:446:ILE:HG13	2.08	0.54
1:A:86:LEU:HD21	1:A:278:GLU:OE1	2.07	0.53
1:B:135:GLN:O	1:B:139:LEU:HB2	2.08	0.53
1:E:92:THR:OG1	1:E:251:HIS:HE1	1.92	0.53
1:A:55:LEU:HB2	1:A:441:PHE:HE2	1.73	0.53
1:D:42:LEU:O	1:D:45:VAL:HG12	2.09	0.53
1:B:131:ALA:HB2	1:B:234:TRP:NE1	2.14	0.53
1:C:420:GLU:OE1	1:C:422:LYS:HE3	2.09	0.53
1:C:132:ASP:OD1	1:C:134:LYS:HG2	2.09	0.53
1:A:312:ASP:OD2	1:A:316:ARG:NH1	2.42	0.53
1:B:42:LEU:HD12	1:B:44:ARG:CB	2.33	0.53
1:B:85:ARG:NH2	1:B:209:ILE:HD13	2.23	0.53
1:E:127:ASP:CG	1:E:128:THR:N	2.62	0.53
1:A:341:TYR:HA	1:A:345:ALA:HB3	1.91	0.53
1:D:139:LEU:HD23	1:D:234:TRP:CH2	2.44	0.53
1:D:176:ARG:HH12	1:E:357:ASN:HD21	1.56	0.53
1:B:167:ARG:HG2	1:B:167:ARG:HH21	1.74	0.53
1:C:405:LEU:HD23	1:C:405:LEU:C	2.29	0.53
1:A:420:GLU:CD	1:A:422:LYS:HE2	2.30	0.52
1:D:379:LYS:HG3	5:D:722:HOH:O	2.08	0.52
1:D:56:ALA:O	1:D:60:LEU:HD23	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:44:ARG:HH11	1:B:455:TYR:HE2	1.57	0.52
1:A:63:THR:O	1:A:67:GLN:HG3	2.09	0.52
1:A:207:ARG:HA	5:A:625:HOH:O	2.10	0.52
1:D:136:LEU:O	1:D:140:GLN:HG3	2.09	0.52
1:C:379:LYS:HE3	5:C:480:HOH:O	2.10	0.52
1:C:256:PRO:HG2	1:C:307:THR:HG22	1.91	0.52
1:C:42:LEU:HD22	1:C:42:LEU:N	2.22	0.52
1:A:357:ASN:ND2	1:C:176:ARG:HH22	2.08	0.52
1:C:210:THR:HG22	5:C:750:HOH:O	2.09	0.52
1:C:92:THR:OG1	1:C:251:HIS:HE1	1.93	0.52
1:E:156:LEU:HD13	1:E:327:VAL:CG2	2.39	0.52
1:B:310:ARG:O	1:B:314:GLU:HG3	2.08	0.52
1:B:46:VAL:HG12	1:B:46:VAL:O	2.10	0.52
1:F:295:THR:O	1:F:295:THR:HG22	2.10	0.52
1:A:131:ALA:C	1:A:133:GLU:H	2.13	0.51
1:D:447:LEU:CD1	1:F:450:LEU:HB3	2.40	0.51
1:C:63:THR:O	1:C:66:ILE:HG12	2.09	0.51
1:F:63:THR:O	1:F:67:GLN:HG3	2.11	0.51
1:D:44:ARG:HD2	1:D:455:TYR:CE2	2.45	0.51
1:F:312:ASP:HB3	5:F:687:HOH:O	2.11	0.51
1:D:440:LEU:HD23	1:F:443:GLY:HA3	1.93	0.51
1:D:274:VAL:HG22	1:D:375:LEU:HG	1.92	0.51
1:E:271:GLN:HE21	1:F:243:GLU:HG2	1.74	0.51
1:E:327:VAL:HG12	5:E:480:HOH:O	2.09	0.51
1:E:114:GLU:HG2	1:E:342:LYS:HE3	1.93	0.51
1:B:271:GLN:HE21	1:C:243:GLU:HG2	1.76	0.51
1:A:120:ASN:ND2	1:A:122:ARG:H	2.08	0.51
1:B:319:VAL:O	1:B:323:ASN:HA	2.11	0.51
1:D:209:ILE:C	1:D:209:ILE:HD12	2.31	0.51
1:E:85:ARG:NH2	1:E:85:ARG:HB3	2.26	0.51
1:A:256:PRO:HG2	1:A:307:THR:HG22	1.92	0.51
1:D:256:PRO:HG2	1:D:307:THR:HG22	1.92	0.51
1:C:446:ILE:HG22	1:C:450:LEU:HD22	1.93	0.50
1:C:310:ARG:O	1:C:314:GLU:HG3	2.11	0.50
1:E:418:THR:HG23	5:E:543:HOH:O	2.12	0.50
1:D:202:GLN:C	1:D:204:GLY:H	2.14	0.50
1:A:402:GLU:OE1	1:C:383:LYS:HE2	2.11	0.50
1:C:205:LYS:H	1:C:206:PRO:HD2	1.77	0.50
1:B:294:THR:HG21	1:B:303:THR:HA	1.93	0.50
1:C:287:PRO:HG2	5:C:727:HOH:O	2.10	0.50
1:B:454:ASP:OD2	1:C:40:LEU:HD21	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:442:ILE:O	1:C:446:ILE:HG13	2.11	0.50
1:D:446:ILE:HG13	1:E:54:SER:HB2	1.94	0.50
1:F:75:VAL:HG13	1:F:422:LYS:HB2	1.93	0.50
1:A:292:LYS:HA	5:A:644:HOH:O	2.12	0.50
1:A:298:SER:HB2	1:A:301:TYR:C	2.32	0.50
1:D:186:LYS:HE3	5:D:697:HOH:O	2.12	0.50
1:A:43:LYS:NZ	1:A:43:LYS:HB3	2.27	0.50
1:A:144:ASN:HD21	1:A:146:ARG:HE	1.60	0.50
1:C:395:LYS:HG2	1:C:399:TYR:CE1	2.47	0.49
1:A:205:LYS:O	1:A:207:ARG:N	2.45	0.49
1:C:420:GLU:CD	1:C:422:LYS:HE3	2.33	0.49
1:A:176:ARG:NH1	1:B:357:ASN:HD21	2.09	0.49
1:C:154:ASN:ND2	1:C:156:LEU:HB3	2.27	0.49
1:C:293:ALA:C	1:C:295:THR:H	2.16	0.49
1:B:176:ARG:HH22	1:C:357:ASN:ND2	2.10	0.49
1:F:346:ASP:HB2	1:F:347:PRO:HD3	1.95	0.49
1:E:202:GLN:HB2	1:E:205:LYS:CG	2.42	0.49
1:B:210:THR:HG23	1:B:217:ASN:HB3	1.95	0.49
1:C:274:VAL:HG22	1:C:375:LEU:HG	1.95	0.49
1:B:438:MET:O	1:B:442:ILE:HG13	2.13	0.49
1:D:282:ILE:HB	1:D:420:GLU:HG3	1.95	0.49
1:B:274:VAL:HG22	1:B:375:LEU:HG	1.95	0.49
1:B:136:LEU:O	1:B:140:GLN:HG3	2.13	0.48
1:C:42:LEU:H	1:C:42:LEU:CD2	2.23	0.48
1:F:101:PHE:CE1	1:F:139:LEU:HD21	2.47	0.48
1:D:209:ILE:HD12	1:D:209:ILE:O	2.13	0.48
1:C:44:ARG:CZ	1:C:455:TYR:HB2	2.43	0.48
1:D:445:SER:O	1:D:449:VAL:HG23	2.13	0.48
1:D:202:GLN:HG3	5:D:697:HOH:O	2.13	0.48
1:D:390:ALA:HB1	1:D:395:LYS:O	2.14	0.48
1:F:452:LEU:HD13	1:F:452:LEU:O	2.13	0.48
1:A:387:LYS:HE2	1:A:397:GLU:OE2	2.13	0.48
1:C:292:LYS:HD2	1:C:363:GLU:OE1	2.13	0.48
1:A:400:ILE:HG23	1:A:404:ILE:HG13	1.95	0.48
1:E:51:PHE:HD2	1:E:447:LEU:HD13	1.77	0.48
1:D:122:ARG:O	1:D:124:GLU:HG3	2.14	0.48
1:A:387:LYS:HD3	5:A:747:HOH:O	2.12	0.48
1:D:211:MET:HG3	1:E:357:ASN:HD22	1.74	0.48
1:D:116:LEU:HA	5:D:705:HOH:O	2.12	0.48
1:B:292:LYS:O	1:B:292:LYS:HG3	2.13	0.48
1:B:44:ARG:NH1	1:B:455:TYR:HE2	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:395:LYS:HE3	5:C:635:HOH:O	2.13	0.48
1:B:346:ASP:HB2	1:B:347:PRO:HD3	1.96	0.48
1:F:85:ARG:HD3	1:F:209:ILE:HD12	1.96	0.48
1:E:339:GLU:HG3	5:E:694:HOH:O	2.13	0.48
1:E:202:GLN:HB2	1:E:205:LYS:HG2	1.95	0.47
1:E:78:LEU:HD13	1:E:419:ILE:HG12	1.96	0.47
1:A:395:LYS:HG2	1:A:399:TYR:CE1	2.48	0.47
1:D:49:LEU:HD12	1:D:50:CYS:N	2.28	0.47
1:A:78:LEU:HD13	1:A:78:LEU:C	2.34	0.47
1:A:176:ARG:HH22	1:B:357:ASN:HD21	1.58	0.47
1:E:101:PHE:CE1	1:E:139:LEU:HD21	2.50	0.47
1:B:236:GLU:HG2	1:B:242:PHE:HZ	1.80	0.47
1:D:436:GLY:O	1:D:440:LEU:HD13	2.14	0.47
1:F:97:ASN:ND2	1:F:231:LEU:H	2.10	0.47
1:F:55:LEU:C	1:F:55:LEU:HD13	2.34	0.47
1:C:207:ARG:HA	5:C:639:HOH:O	2.14	0.47
1:F:292:LYS:HD2	1:F:304:TYR:CD2	2.50	0.47
1:E:442:ILE:C	1:E:444:ALA:H	2.18	0.47
1:B:85:ARG:HG2	1:B:209:ILE:HD12	1.97	0.47
1:B:456:ALA:O	1:B:459:VAL:HG23	2.15	0.47
1:D:92:THR:OG1	1:D:251:HIS:HE1	1.96	0.47
1:E:59:ALA:O	1:E:63:THR:HG23	2.15	0.47
1:D:420:GLU:OE1	1:D:422:LYS:HE2	2.15	0.47
1:D:435:GLY:HA3	1:E:61:VAL:HG11	1.97	0.47
1:E:75:VAL:HG23	1:E:424:ALA:HB2	1.96	0.47
1:D:181:SER:HB2	1:D:182:PRO:CD	2.45	0.47
1:A:170:LEU:HD11	1:A:173:CYS:HB2	1.97	0.47
1:F:52:MET:O	1:F:55:LEU:HB3	2.13	0.46
1:C:205:LYS:H	1:C:206:PRO:CD	2.27	0.46
1:B:207:ARG:HH21	1:B:207:ARG:CB	2.20	0.46
1:E:299:GLU:C	1:E:301:TYR:H	2.18	0.46
1:B:97:ASN:ND2	1:B:231:LEU:H	2.09	0.46
1:F:315:THR:O	1:F:319:VAL:HG23	2.15	0.46
3:C:6:NAG:H83	3:C:6:NAG:O3	2.15	0.46
1:F:434:ILE:HG22	1:F:438:MET:HE2	1.98	0.46
1:C:427:VAL:O	1:C:431:LEU:HD13	2.14	0.46
1:B:452:LEU:HA	1:B:455:TYR:HB3	1.96	0.46
1:F:45:VAL:HG23	1:F:46:VAL:N	2.30	0.46
1:A:149:LYS:O	1:A:151:LYS:HD3	2.16	0.46
1:C:47:TRP:CZ3	1:C:447:LEU:HB3	2.51	0.46
1:D:120:ASN:HD21	1:D:124:GLU:H	1.64	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:181:SER:HB2	1:E:182:PRO:CD	2.46	0.46
1:A:120:ASN:ND2	1:A:124:GLU:H	2.14	0.46
1:F:442:ILE:O	1:F:446:ILE:HG13	2.15	0.46
1:C:42:LEU:O	1:C:45:VAL:HG22	2.16	0.46
1:D:46:VAL:HA	1:D:49:LEU:HG	1.98	0.46
1:E:434:ILE:HA	1:E:437:GLN:HB3	1.98	0.46
1:C:448:THR:HG23	1:C:452:LEU:HD12	1.98	0.46
1:B:53:GLY:O	1:B:57:LEU:HD23	2.15	0.46
1:E:65:ARG:NH2	1:E:433:ASP:HB3	2.28	0.46
1:A:453:PHE:HE1	1:B:43:LYS:HZ2	1.64	0.46
1:C:62:CYS:O	1:C:66:ILE:HG23	2.16	0.46
1:B:101:PHE:CE1	1:B:139:LEU:HD13	2.51	0.45
1:B:405:LEU:O	1:B:405:LEU:HD23	2.17	0.45
1:A:205:LYS:HA	1:A:206:PRO:HD2	1.80	0.45
1:A:201:GLY:O	1:A:202:GLN:HB2	2.16	0.45
3:D:7:NAG:H83	3:D:7:NAG:O3	2.17	0.45
1:A:240:THR:HG22	5:A:618:HOH:O	2.16	0.45
1:D:49:LEU:C	1:D:49:LEU:HD12	2.37	0.45
1:F:282:ILE:HB	1:F:420:GLU:HG3	1.98	0.45
1:D:74:HIS:HD2	5:D:588:HOH:O	1.99	0.45
1:C:89:PRO:HB3	1:C:371:TYR:CZ	2.51	0.45
1:C:139:LEU:HD23	1:C:234:TRP:CH2	2.51	0.45
1:E:282:ILE:HB	1:E:420:GLU:HG3	1.98	0.45
1:A:63:THR:O	1:A:66:ILE:HG22	2.17	0.45
1:C:137:GLU:HG2	5:C:632:HOH:O	2.17	0.45
1:A:390:ALA:HB1	1:A:395:LYS:O	2.15	0.45
1:E:420:GLU:CD	1:E:422:LYS:HD3	2.37	0.45
1:D:446:ILE:O	1:D:450:LEU:HG	2.17	0.45
1:A:58:LEU:HD13	1:A:438:MET:HA	1.99	0.45
1:E:132:ASP:OD2	1:E:134:LYS:HB3	2.17	0.45
1:B:181:SER:HB2	1:B:182:PRO:CD	2.47	0.45
1:D:280:ARG:HG3	1:D:416:TYR:CE1	2.51	0.45
1:B:61:VAL:HG11	1:B:437:GLN:HG2	1.97	0.45
1:C:205:LYS:HB3	1:C:206:PRO:HD3	1.97	0.45
1:A:227:GLN:HA	1:A:230:TYR:CD1	2.52	0.45
1:F:192:TYR:CE2	1:F:260:ASP:HA	2.52	0.45
1:A:176:ARG:NH2	1:B:357:ASN:HD21	2.15	0.45
1:C:154:ASN:HD21	1:C:156:LEU:HB3	1.82	0.45
1:E:97:ASN:ND2	1:E:231:LEU:H	2.13	0.45
1:B:436:GLY:O	1:B:440:LEU:HG	2.17	0.45
1:E:129:GLN:C	1:E:131:ALA:H	2.20	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:130:THR:HG22	1:E:130:THR:O	2.17	0.45
1:B:434:ILE:O	1:B:438:MET:HG2	2.17	0.45
1:A:204:GLY:O	1:A:206:PRO:N	2.49	0.44
1:F:274:VAL:HG22	1:F:375:LEU:HG	1.99	0.44
1:E:300:PHE:HD2	1:E:312:ASP:CG	2.21	0.44
1:F:395:LYS:HG2	1:F:399:TYR:CD1	2.51	0.44
1:E:53:GLY:C	1:E:55:LEU:N	2.70	0.44
1:B:449:VAL:HA	1:B:452:LEU:CD2	2.47	0.44
1:E:53:GLY:O	1:E:54:SER:HB3	2.18	0.44
1:C:43:LYS:O	1:C:47:TRP:HD1	2.00	0.44
1:D:132:ASP:HB2	5:D:651:HOH:O	2.17	0.44
1:F:433:ASP:O	1:F:437:GLN:HG2	2.17	0.44
1:D:405:LEU:HD12	1:D:405:LEU:C	2.38	0.44
1:A:134:LYS:O	1:A:138:ILE:HG22	2.18	0.44
1:D:176:ARG:HH22	1:E:357:ASN:HD21	1.60	0.44
1:E:51:PHE:HB2	1:E:448:THR:OG1	2.17	0.44
1:E:405:LEU:HD12	1:E:405:LEU:C	2.38	0.44
1:E:133:GLU:HG3	1:E:134:LYS:N	2.33	0.44
1:C:109:LEU:HG	1:C:119:LEU:HD11	1.99	0.44
1:F:434:ILE:HG22	1:F:438:MET:CE	2.48	0.44
1:D:84:THR:O	1:D:85:ARG:HB2	2.17	0.44
1:A:53:GLY:O	1:A:57:LEU:HD23	2.17	0.44
1:C:42:LEU:O	1:C:46:VAL:HG23	2.17	0.44
1:E:55:LEU:HD11	1:E:58:LEU:HD22	2.00	0.44
1:A:295:THR:CG2	1:A:296:GLY:N	2.81	0.43
1:F:120:ASN:ND2	1:F:124:GLU:H	2.17	0.43
1:D:227:GLN:HA	1:D:230:TYR:CD1	2.53	0.43
1:E:353:VAL:HG23	1:E:354:GLU:HG3	2.01	0.43
1:F:42:LEU:O	1:F:42:LEU:HD22	2.19	0.43
1:E:58:LEU:HD12	1:E:58:LEU:N	2.34	0.43
1:C:346:ASP:HB2	1:C:347:PRO:HD3	2.00	0.43
1:D:395:LYS:HG2	1:D:399:TYR:CE1	2.54	0.43
1:B:120:ASN:ND2	1:B:120:ASN:C	2.70	0.43
1:E:271:GLN:NE2	1:F:243:GLU:HG2	2.33	0.43
1:F:55:LEU:HD22	1:F:55:LEU:O	2.18	0.43
1:D:43:LYS:HB3	1:D:43:LYS:HZ3	1.84	0.43
1:F:227:GLN:HA	1:F:230:TYR:CD1	2.54	0.43
1:B:395:LYS:HG2	1:B:399:TYR:CE1	2.53	0.43
1:B:165:ASP:OD1	1:B:167:ARG:HG3	2.18	0.43
1:F:300:PHE:HD2	1:F:312:ASP:OD1	2.01	0.43
1:C:293:ALA:O	1:C:295:THR:N	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:445:SER:O	1:A:449:VAL:HG23	2.18	0.43
1:B:45:VAL:O	1:B:49:LEU:HG	2.19	0.43
1:E:181:SER:HB2	1:E:182:PRO:HD2	2.01	0.43
1:E:135:GLN:NE2	1:E:232:PRO:HG3	2.34	0.43
1:D:271:GLN:HE21	1:E:243:GLU:HG2	1.84	0.43
1:B:139:LEU:HA	1:B:139:LEU:HD12	1.86	0.43
1:A:131:ALA:C	1:A:133:GLU:N	2.71	0.43
1:C:128:THR:HB	1:C:234:TRP:CE2	2.53	0.43
1:D:346:ASP:HB2	1:D:347:PRO:HD3	2.01	0.43
1:F:43:LYS:NZ	1:F:43:LYS:HB3	2.34	0.43
1:E:98:GLU:HG2	1:E:192:TYR:O	2.19	0.43
1:F:427:VAL:O	1:F:431:LEU:HD13	2.20	0.42
1:B:449:VAL:O	1:B:453:PHE:HB2	2.20	0.42
1:B:126:PRO:O	1:B:127:ASP:C	2.58	0.42
1:C:205:LYS:N	1:C:206:PRO:CD	2.81	0.42
1:D:176:ARG:NH1	1:E:357:ASN:HD21	2.17	0.42
1:B:121:ASN:C	1:B:121:ASN:HD22	2.22	0.42
1:D:427:VAL:O	1:D:431:LEU:HD13	2.18	0.42
1:C:280:ARG:HG2	1:C:280:ARG:HH11	1.84	0.42
1:D:106:LYS:HE3	1:D:106:LYS:HB2	1.88	0.42
1:F:292:LYS:HD3	1:F:292:LYS:C	2.40	0.42
1:B:45:VAL:C	1:B:47:TRP:N	2.72	0.42
1:D:447:LEU:HD13	1:D:447:LEU:O	2.19	0.42
1:E:268:PRO:HA	1:E:405:LEU:HB3	2.01	0.42
1:A:346:ASP:N	1:A:347:PRO:HD2	2.34	0.42
1:F:339:GLU:H	1:F:339:GLU:CD	2.23	0.42
1:B:135:GLN:O	1:B:138:ILE:HG23	2.19	0.42
1:B:134:LYS:O	1:B:138:ILE:HG22	2.19	0.42
1:B:121:ASN:ND2	1:B:122:ARG:HG3	2.33	0.42
1:D:146:ARG:HH11	1:D:146:ARG:HG3	1.84	0.42
1:A:256:PRO:O	1:A:307:THR:HG21	2.19	0.42
1:F:201:GLY:O	1:F:202:GLN:NE2	2.53	0.42
1:D:241:SER:HB2	5:D:518:HOH:O	2.19	0.42
1:E:58:LEU:O	1:E:62:CYS:HB2	2.20	0.42
1:B:394:ASN:O	1:B:395:LYS:HD2	2.18	0.42
1:B:227:GLN:HA	1:B:230:TYR:CD1	2.55	0.42
1:B:120:ASN:ND2	1:B:124:GLU:H	2.17	0.42
1:F:47:TRP:HH2	1:F:448:THR:HG1	1.60	0.42
1:A:405:LEU:C	1:A:405:LEU:HD12	2.40	0.42
1:D:55:LEU:HB2	1:D:441:PHE:HE2	1.84	0.42
1:C:85:ARG:HH21	1:C:209:ILE:HD13	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:97:ASN:ND2	1:A:231:LEU:H	2.14	0.42
1:D:202:GLN:OE1	1:D:202:GLN:HA	2.20	0.42
1:B:454:ASP:OD1	1:C:40:LEU:HD21	2.20	0.41
1:D:46:VAL:O	1:D:49:LEU:HG	2.19	0.41
1:B:128:THR:O	1:B:130:THR:N	2.53	0.41
1:D:64:ASN:OD1	1:D:65:ARG:HD2	2.20	0.41
1:F:181:SER:HB3	1:F:182:PRO:CD	2.50	0.41
1:B:448:THR:O	1:B:452:LEU:HD22	2.20	0.41
1:B:42:LEU:CD1	1:B:44:ARG:HB2	2.38	0.41
1:D:126:PRO:O	1:D:127:ASP:C	2.59	0.41
5:A:728:HOH:O	1:B:437:GLN:HG3	2.19	0.41
1:F:374:GLU:HB3	5:F:591:HOH:O	2.19	0.41
1:D:97:ASN:ND2	1:D:231:LEU:H	2.16	0.41
1:D:54:SER:OG	1:D:441:PHE:HA	2.20	0.41
1:B:44:ARG:O	1:B:47:TRP:HB3	2.21	0.41
1:A:173:CYS:C	1:A:180:CYS:SG	2.99	0.41
1:C:227:GLN:HA	1:C:230:TYR:CD1	2.55	0.41
1:E:173:CYS:C	1:E:180:CYS:SG	2.99	0.41
1:A:235:GLY:O	1:A:240:THR:HG21	2.20	0.41
1:C:85:ARG:HD3	1:C:209:ILE:CD1	2.50	0.41
1:D:128:THR:HG22	1:D:129:GLN:N	2.36	0.41
1:A:364:MET:HA	1:A:365:PRO:HD3	1.97	0.41
1:B:188:VAL:HG13	1:B:188:VAL:O	2.21	0.41
1:E:176:ARG:NH1	1:F:357:ASN:HD21	2.17	0.41
1:D:44:ARG:HH11	1:D:44:ARG:HG2	1.85	0.41
1:E:270:PHE:CG	1:E:377:MET:HE3	2.56	0.41
1:A:450:LEU:HD11	1:B:50:CYS:SG	2.61	0.41
1:F:204:GLY:N	5:F:654:HOH:O	2.54	0.41
1:B:295:THR:CG2	1:B:296:GLY:N	2.83	0.41
1:E:306:ILE:O	1:E:310:ARG:HG3	2.20	0.41
1:F:120:ASN:HD22	1:F:122:ARG:H	1.67	0.41
1:A:99:PHE:CE2	1:A:116:LEU:HD21	2.55	0.41
1:E:379:LYS:HD2	1:E:380:ILE:N	2.36	0.41
1:E:72:TYR:HB3	1:E:288:TRP:CD1	2.56	0.41
1:B:292:LYS:HD2	1:B:304:TYR:CZ	2.55	0.41
1:A:144:ASN:OD1	1:A:146:ARG:HG2	2.21	0.41
1:C:433:ASP:O	1:C:437:GLN:HG2	2.21	0.41
1:C:55:LEU:C	1:C:55:LEU:HD13	2.41	0.41
1:A:181:SER:HB2	1:A:182:PRO:HD2	2.03	0.41
1:D:236:GLU:OE1	1:F:392:LYS:NZ	2.44	0.41
1:C:210:THR:HG21	5:C:738:HOH:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:301:TYR:OH	1:A:311:ILE:HG21	2.19	0.41
1:B:67:GLN:HB2	1:B:67:GLN:HE21	1.67	0.41
1:E:55:LEU:CD1	1:E:58:LEU:HD22	2.51	0.40
1:F:181:SER:HB3	1:F:182:PRO:HD2	2.01	0.40
1:F:379:LYS:HD3	5:F:757:HOH:O	2.21	0.40
1:E:431:LEU:HD12	1:E:431:LEU:N	2.36	0.40
1:E:128:THR:HA	1:E:136:LEU:CD2	2.50	0.40
1:D:439:GLY:HA3	1:E:58:LEU:CD1	2.52	0.40
1:F:448:THR:O	1:F:452:LEU:HB2	2.21	0.40
1:A:57:LEU:HB3	1:A:437:GLN:OE1	2.21	0.40
1:E:280:ARG:HG2	1:E:280:ARG:HH21	1.86	0.40
1:A:236:GLU:HG2	1:A:242:PHE:CZ	2.55	0.40
1:B:135:GLN:HA	1:B:138:ILE:CG2	2.52	0.40
1:D:357:ASN:HD21	1:F:176:ARG:NH1	2.19	0.40
1:E:52:MET:HG3	1:E:448:THR:OG1	2.21	0.40
1:B:387:LYS:HE2	1:C:131:ALA:HA	2.04	0.40
1:D:176:ARG:NH2	1:E:357:ASN:HD21	2.20	0.40
1:B:104:VAL:HG21	1:B:231:LEU:HD21	2.03	0.40
1:B:303:THR:HG22	1:B:304:TYR:N	2.37	0.40
1:E:44:ARG:HG2	1:E:44:ARG:HH21	1.87	0.40
1:C:85:ARG:HD3	1:C:209:ILE:HD12	2.03	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	415/438 (95%)	396 (95%)	12 (3%)	7 (2%)	11 2
1	B	418/438 (95%)	397 (95%)	18 (4%)	3 (1%)	26 14
1	C	416/438 (95%)	398 (96%)	12 (3%)	6 (1%)	14 4
1	D	413/438 (94%)	390 (94%)	18 (4%)	5 (1%)	16 5

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	E	419/438 (96%)	397 (95%)	20 (5%)	2 (0%)	34 21
1	F	410/438 (94%)	394 (96%)	13 (3%)	3 (1%)	26 14
All	All	2491/2628 (95%)	2372 (95%)	93 (4%)	26 (1%)	19 7

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	202	GLN
1	A	203	ASP
1	A	206	PRO
1	C	205	LYS
1	D	132	ASP
1	D	298	SER
1	D	299	GLU
1	E	127	ASP
1	F	43	LYS
1	D	127	ASP
1	F	299	GLU
1	A	207	ARG
1	B	46	VAL
1	B	129	GLN
1	C	286	PRO
1	C	294	THR
1	C	455	TYR
1	F	297	ASP
1	A	205	LYS
1	C	206	PRO
1	C	297	ASP
1	E	435	GLY
1	A	296	GLY
1	B	126	PRO
1	D	126	PRO
1	A	126	PRO

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	363/383 (95%)	351 (97%)	12 (3%)	45	34
1	B	366/383 (96%)	354 (97%)	12 (3%)	45	34
1	C	364/383 (95%)	358 (98%)	6 (2%)	70	66
1	D	361/383 (94%)	355 (98%)	6 (2%)	68	64
1	E	367/383 (96%)	358 (98%)	9 (2%)	55	47
1	F	359/383 (94%)	346 (96%)	13 (4%)	42	30
All	All	2180/2298 (95%)	2122 (97%)	58 (3%)	52	43

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	42	LEU
1	A	120	ASN
1	A	147	ASN
1	A	151	LYS
1	A	180	CYS
1	A	217	ASN
1	A	240	THR
1	A	299	GLU
1	A	302	ASP
1	A	381	PRO
1	A	430	LEU
1	A	457	TYR
1	B	42	LEU
1	B	120	ASN
1	B	121	ASN
1	B	180	CYS
1	B	207	ARG
1	B	217	ASN
1	B	290	ASP
1	B	312	ASP
1	B	320	GLU
1	B	405	LEU
1	B	437	GLN
1	B	458	GLU
1	C	180	CYS
1	C	202	GLN
1	C	217	ASN
1	C	405	LEU
1	C	450	LEU
1	C	457	TYR

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Mol	Chain	Res	Type
1	D	120	ASN
1	D	139	LEU
1	D	180	CYS
1	D	312	ASP
1	D	341	TYR
1	D	367	ASN
1	E	122	ARG
1	E	180	CYS
1	E	217	ASN
1	E	292	LYS
1	E	379	LYS
1	E	430	LEU
1	E	447	LEU
1	E	453	PHE
1	E	458	GLU
1	F	42	LEU
1	F	47	TRP
1	F	55	LEU
1	F	120	ASN
1	F	129	GLN
1	F	180	CYS
1	F	217	ASN
1	F	231	LEU
1	F	292	LYS
1	F	381	PRO
1	F	395	LYS
1	F	451	GLU
1	F	452	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (49) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	97	ASN
1	A	111	HIS
1	A	120	ASN
1	A	129	GLN
1	A	154	ASN
1	A	202	GLN
1	A	357	ASN
1	A	437	GLN
1	B	67	GLN
1	B	97	ASN

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Mol	Chain	Res	Type
1	B	120	ASN
1	B	121	ASN
1	B	147	ASN
1	B	251	HIS
1	B	271	GLN
1	B	321	ASN
1	B	323	ASN
1	B	357	ASN
1	B	437	GLN
1	C	64	ASN
1	C	97	ASN
1	C	154	ASN
1	C	202	GLN
1	C	251	HIS
1	C	321	ASN
1	C	357	ASN
1	D	74	HIS
1	D	97	ASN
1	D	120	ASN
1	D	135	GLN
1	D	147	ASN
1	D	251	HIS
1	D	271	GLN
1	D	357	ASN
1	E	67	GLN
1	E	97	ASN
1	E	135	GLN
1	E	251	HIS
1	E	271	GLN
1	E	357	ASN
1	E	398	GLN
1	F	64	ASN
1	F	67	GLN
1	F	97	ASN
1	F	120	ASN
1	F	251	HIS
1	F	323	ASN
1	F	357	ASN
1	F	398	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 21 ligands modelled in this entry, 6 are monoatomic - leaving 15 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	NAG	A	1	1	14,14,15	0.48	0	15,19,21	0.76	1 (6%)
3	NAG	A	2	1	14,14,15	0.58	0	15,19,21	0.73	1 (6%)
2	MAL	B	1	-	24,24,24	0.95	0	35,35,35	0.97	1 (2%)
2	MAL	B	2	-	24,24,24	0.98	1 (4%)	35,35,35	0.92	1 (2%)
3	NAG	B	3	1	14,14,15	0.49	0	15,19,21	0.75	1 (6%)
3	NAG	B	4	1	14,14,15	0.50	0	15,19,21	0.64	0
2	MAL	C	3	-	24,24,24	0.97	1 (4%)	35,35,35	0.95	1 (2%)
3	NAG	C	5	1	14,14,15	0.51	0	15,19,21	0.61	0
3	NAG	C	6	1	14,14,15	0.52	0	15,19,21	0.68	1 (6%)
3	NAG	D	7	1	14,14,15	0.48	0	15,19,21	0.75	1 (6%)
3	NAG	D	8	1	14,14,15	0.59	0	15,19,21	0.76	1 (6%)
3	NAG	E	10	1	14,14,15	0.51	0	15,19,21	0.71	1 (6%)
3	NAG	E	9	1	14,14,15	0.48	0	15,19,21	0.75	1 (6%)
3	NAG	F	11	1	14,14,15	0.54	0	15,19,21	0.68	1 (6%)
3	NAG	F	12	1	14,14,15	0.57	0	15,19,21	0.64	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	A	1	1	-	0/6/23/26	0/1/1/1
3	NAG	A	2	1	-	0/6/23/26	0/1/1/1
2	MAL	B	1	-	-	0/8/48/48	0/2/2/2
2	MAL	B	2	-	-	0/8/48/48	0/2/2/2
3	NAG	B	3	1	-	0/6/23/26	0/1/1/1
3	NAG	B	4	1	-	0/6/23/26	0/1/1/1
2	MAL	C	3	-	-	0/8/48/48	0/2/2/2
3	NAG	C	5	1	-	0/6/23/26	0/1/1/1
3	NAG	C	6	1	-	0/6/23/26	0/1/1/1
3	NAG	D	7	1	-	0/6/23/26	0/1/1/1
3	NAG	D	8	1	-	0/6/23/26	0/1/1/1
3	NAG	E	10	1	-	0/6/23/26	0/1/1/1
3	NAG	E	9	1	-	0/6/23/26	0/1/1/1
3	NAG	F	11	1	-	0/6/23/26	0/1/1/1
3	NAG	F	12	1	-	0/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2	MAL	O5-C1	2.09	1.47	1.41
2	C	3	MAL	O5-C1	2.09	1.47	1.41

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1	MAL	C1-O1-C4'	-3.79	108.11	118.01
2	C	3	MAL	C1-O1-C4'	-3.70	108.33	118.01
2	B	2	MAL	C1-O1-C4'	-3.42	109.08	118.01
3	D	8	NAG	C2-N2-C7	-2.43	119.92	123.04
3	E	9	NAG	C2-N2-C7	-2.42	119.93	123.04
3	A	1	NAG	C2-N2-C7	-2.40	119.96	123.04
3	D	7	NAG	C2-N2-C7	-2.37	119.99	123.04
3	B	3	NAG	C2-N2-C7	-2.28	120.11	123.04
3	A	2	NAG	C2-N2-C7	-2.27	120.13	123.04
3	E	10	NAG	C2-N2-C7	-2.14	120.29	123.04
3	F	11	NAG	C2-N2-C7	-2.08	120.36	123.04
3	C	6	NAG	C2-N2-C7	-2.05	120.41	123.04

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	6	NAG	1	0
3	D	7	NAG	1	0
3	F	11	NAG	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å^2)	Q<0.9
1	A	417/438 (95%)	0.76	57 (13%)	4 4	13, 30, 80, 91	0
1	B	420/438 (95%)	0.72	53 (12%)	5 5	12, 31, 85, 97	0
1	C	418/438 (95%)	0.52	43 (10%)	9 9	13, 28, 73, 88	0
1	D	415/438 (94%)	0.96	79 (19%)	2 2	12, 31, 80, 91	0
1	E	421/438 (96%)	1.03	69 (16%)	2 2	11, 31, 87, 96	0
1	F	412/438 (94%)	0.88	70 (16%)	2 2	13, 30, 81, 94	0
All	All	2503/2628 (95%)	0.81	371 (14%)	3 3	11, 30, 82, 97	0

All (371) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	42	LEU	15.1
1	B	296	GLY	14.3
1	B	453	PHE	13.1
1	A	295	THR	12.4
1	E	294	THR	12.2
1	D	128	THR	11.5
1	A	297	ASP	11.3
1	D	297	ASP	11.2
1	B	295	THR	11.1
1	E	298	SER	11.1
1	D	45	VAL	11.0
1	E	457	TYR	10.7
1	E	54	SER	10.1
1	D	294	THR	10.0
1	E	48	ALA	10.0
1	F	298	SER	10.0
1	C	457	TYR	9.9
1	D	293	ALA	9.8
1	D	296	GLY	9.8

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Mol	Chain	Res	Type	RSRZ
1	D	295	THR	9.7
1	F	293	ALA	9.7
1	B	128	THR	9.7
1	F	295	THR	9.7
1	E	297	ASP	9.5
1	E	295	THR	9.4
1	D	453	PHE	9.4
1	B	457	TYR	9.3
1	E	42	LEU	9.3
1	D	129	GLN	9.3
1	F	452	LEU	9.0
1	A	298	SER	8.8
1	F	296	GLY	8.8
1	F	297	ASP	8.8
1	B	298	SER	8.7
1	A	455	TYR	8.7
1	E	128	THR	8.6
1	C	295	THR	8.6
1	A	206	PRO	8.5
1	A	453	PHE	8.5
1	F	202	GLN	8.5
1	A	296	GLY	8.4
1	A	457	TYR	8.3
1	C	293	ALA	8.3
1	B	297	ASP	8.2
1	E	453	PHE	8.1
1	A	132	ASP	8.0
1	F	294	THR	8.0
1	C	297	ASP	8.0
1	F	450	LEU	8.0
1	F	300	PHE	7.9
1	C	296	GLY	7.9
1	E	460	ILE	7.8
1	E	296	GLY	7.8
1	F	45	VAL	7.7
1	E	50	CYS	7.6
1	B	300	PHE	7.6
1	E	452	LEU	7.6
1	E	293	ALA	7.6
1	A	203	ASP	7.5
1	A	294	THR	7.5
1	C	298	SER	7.2

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Mol	Chain	Res	Type	RSRZ
1	B	45	VAL	7.1
1	E	446	ILE	7.1
1	F	299	GLU	7.0
1	B	294	THR	6.8
1	A	204	GLY	6.7
1	A	456	ALA	6.7
1	E	55	LEU	6.7
1	D	452	LEU	6.7
1	D	455	TYR	6.6
1	F	301	TYR	6.6
1	B	42	LEU	6.6
1	D	447	LEU	6.6
1	D	454	ASP	6.5
1	E	51	PHE	6.5
1	E	52	MET	6.4
1	F	44	ARG	6.3
1	D	203	ASP	6.3
1	B	46	VAL	6.3
1	F	204	GLY	6.3
1	E	43	LYS	6.2
1	D	132	ASP	6.2
1	D	202	GLN	6.1
1	A	129	GLN	6.1
1	D	298	SER	6.1
1	F	453	PHE	6.1
1	D	444	ALA	6.0
1	F	446	ILE	5.9
1	C	203	ASP	5.9
1	B	129	GLN	5.9
1	F	449	VAL	5.8
1	E	450	LEU	5.8
1	C	294	THR	5.7
1	D	206	PRO	5.7
1	B	449	VAL	5.7
1	B	459	VAL	5.6
1	E	46	VAL	5.6
1	A	42	LEU	5.6
1	E	133	GLU	5.6
1	C	204	GLY	5.6
1	B	454	ASP	5.6
1	E	49	LEU	5.6
1	D	450	LEU	5.5

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Mol	Chain	Res	Type	RSRZ
1	F	48	ALA	5.5
1	A	205	LYS	5.5
1	E	445	SER	5.5
1	B	52	MET	5.4
1	B	299	GLU	5.3
1	B	460	ILE	5.3
1	E	300	PHE	5.2
1	D	456	ALA	5.2
1	A	47	TRP	5.2
1	A	450	LEU	5.2
1	F	66	ILE	5.2
1	D	448	THR	5.1
1	F	427	VAL	5.1
1	A	127	ASP	5.1
1	A	130	THR	5.1
1	E	45	VAL	5.1
1	F	49	LEU	5.0
1	F	203	ASP	5.0
1	E	444	ALA	5.0
1	C	40	LEU	5.0
1	B	51	PHE	5.0
1	C	205	LYS	5.0
1	D	449	VAL	5.0
1	D	49	LEU	4.9
1	B	452	LEU	4.9
1	C	42	LEU	4.9
1	D	42	LEU	4.8
1	F	127	ASP	4.8
1	A	202	GLN	4.7
1	A	452	LEU	4.7
1	A	449	VAL	4.7
1	C	45	VAL	4.6
1	A	134	LYS	4.6
1	D	52	MET	4.6
1	E	122	ARG	4.6
1	A	128	THR	4.6
1	A	293	ALA	4.6
1	D	127	ASP	4.6
1	D	133	GLU	4.5
1	D	51	PHE	4.5
1	D	146	ARG	4.4
1	E	455	TYR	4.4

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Mol	Chain	Res	Type	RSRZ
1	E	361	VAL	4.4
1	E	458	GLU	4.4
1	F	146	ARG	4.4
1	E	41	SER	4.4
1	E	129	GLN	4.4
1	E	448	THR	4.4
1	C	206	PRO	4.4
1	E	299	GLU	4.4
1	F	441	PHE	4.4
1	E	360	CYS	4.4
1	E	47	TRP	4.3
1	E	447	LEU	4.3
1	E	130	THR	4.3
1	D	47	TRP	4.2
1	B	450	LEU	4.2
1	E	70	PHE	4.2
1	F	133	GLU	4.2
1	F	50	CYS	4.1
1	D	72	TYR	4.1
1	C	286	PRO	4.1
1	D	46	VAL	4.1
1	E	456	ALA	4.0
1	F	128	THR	4.0
1	D	205	LYS	4.0
1	A	45	VAL	4.0
1	B	361	VAL	4.0
1	A	300	PHE	4.0
1	E	438	MET	4.0
1	B	47	TRP	4.0
1	F	47	TRP	4.0
1	E	449	VAL	4.0
1	C	66	ILE	4.0
1	D	53	GLY	3.9
1	D	204	GLY	3.9
1	D	446	ILE	3.9
1	C	300	PHE	3.9
1	B	43	LYS	3.9
1	D	451	GLU	3.9
1	F	70	PHE	3.8
1	F	205	LYS	3.8
1	F	51	PHE	3.8
1	A	141	ASP	3.8

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Mol	Chain	Res	Type	RSRZ
1	F	443	GLY	3.8
1	E	443	GLY	3.8
1	F	46	VAL	3.8
1	B	133	GLU	3.8
1	C	455	TYR	3.7
1	A	46	VAL	3.7
1	B	461	LYS	3.7
1	B	359	TYR	3.7
1	E	359	TYR	3.7
1	E	461	LYS	3.7
1	E	203	ASP	3.7
1	F	302	ASP	3.7
1	F	60	LEU	3.7
1	F	52	MET	3.7
1	B	456	ALA	3.7
1	E	442	ILE	3.7
1	A	299	GLU	3.7
1	E	454	ASP	3.7
1	A	447	LEU	3.7
1	D	134	LYS	3.6
1	A	442	ILE	3.6
1	B	127	ASP	3.6
1	C	44	ARG	3.6
1	C	427	VAL	3.6
1	A	454	ASP	3.6
1	E	62	CYS	3.6
1	C	41	SER	3.5
1	E	301	TYR	3.5
1	C	47	TRP	3.5
1	D	445	SER	3.5
1	C	453	PHE	3.5
1	C	456	ALA	3.5
1	F	57	LEU	3.5
1	D	55	LEU	3.4
1	D	44	ARG	3.4
1	F	206	PRO	3.4
1	D	442	ILE	3.4
1	F	288	TRP	3.4
1	D	286	PRO	3.4
1	F	440	LEU	3.3
1	B	44	ARG	3.3
1	D	48	ALA	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	451	GLU	3.3
1	B	134	LYS	3.3
1	E	459	VAL	3.3
1	F	451	GLU	3.3
1	C	450	LEU	3.2
1	A	146	ARG	3.2
1	E	127	ASP	3.2
1	B	455	TYR	3.2
1	C	359	TYR	3.2
1	A	137	GLU	3.2
1	C	302	ASP	3.2
1	A	131	ALA	3.2
1	E	44	ARG	3.1
1	D	59	ALA	3.1
1	F	71	LEU	3.1
1	A	66	ILE	3.1
1	E	125	ILE	3.1
1	D	299	GLU	3.1
1	D	54	SER	3.1
1	F	43	LYS	3.1
1	A	136	LEU	3.0
1	E	431	LEU	3.0
1	B	332	ASP	3.0
1	A	147	ASN	3.0
1	B	458	GLU	3.0
1	A	44	ARG	3.0
1	D	130	THR	3.0
1	A	133	GLU	3.0
1	C	299	GLU	3.0
1	A	70	PHE	3.0
1	E	292	LYS	3.0
1	D	70	PHE	2.9
1	F	72	TYR	2.9
1	F	56	ALA	2.9
1	D	71	LEU	2.9
1	F	444	ALA	2.9
1	F	431	LEU	2.8
1	B	293	ALA	2.8
1	F	448	THR	2.8
1	A	458	GLU	2.7
1	B	446	ILE	2.7
1	D	126	PRO	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	441	PHE	2.7
1	B	53	GLY	2.7
1	E	439	GLY	2.7
1	F	55	LEU	2.7
1	A	302	ASP	2.7
1	E	302	ASP	2.7
1	D	361	VAL	2.7
1	D	131	ALA	2.7
1	A	43	LYS	2.7
1	A	207	ARG	2.7
1	E	287	PRO	2.7
1	A	60	LEU	2.7
1	F	438	MET	2.6
1	D	145	PHE	2.6
1	E	146	ARG	2.6
1	D	288	TRP	2.6
1	B	287	PRO	2.6
1	C	445	SER	2.6
1	D	359	TYR	2.6
1	F	69	TYR	2.6
1	C	131	ALA	2.6
1	D	274	VAL	2.6
1	D	147	ASN	2.5
1	B	50	CYS	2.5
1	F	447	LEU	2.5
1	C	134	LYS	2.5
1	B	358	GLU	2.5
1	B	55	LEU	2.5
1	D	50	CYS	2.5
1	C	70	PHE	2.5
1	B	132	ASP	2.5
1	F	442	ILE	2.5
1	B	362	CYS	2.5
1	F	439	GLY	2.5
1	A	50	CYS	2.4
1	D	443	GLY	2.4
1	A	122	ARG	2.4
1	B	320	GLU	2.4
1	F	67	GLN	2.4
1	E	72	TYR	2.4
1	E	137	GLU	2.4
1	F	58	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	143	ALA	2.3
1	D	441	PHE	2.3
1	D	61	VAL	2.3
1	C	290	ASP	2.3
1	C	454	ASP	2.3
1	F	375	LEU	2.3
1	F	430	LEU	2.3
1	D	287	PRO	2.3
1	D	43	LYS	2.3
1	D	434	ILE	2.3
1	B	301	TYR	2.3
1	F	147	ASN	2.2
1	A	57	LEU	2.2
1	B	451	GLU	2.2
1	F	274	VAL	2.2
1	F	367	ASN	2.2
1	A	51	PHE	2.2
1	D	292	LYS	2.2
1	D	62	CYS	2.2
1	B	202	GLN	2.2
1	F	426	GLU	2.2
1	B	292	LYS	2.2
1	D	433	ASP	2.2
1	C	438	MET	2.2
1	B	59	ALA	2.2
1	F	286	PRO	2.2
1	F	425	TYR	2.2
1	E	60	LEU	2.2
1	B	219	LEU	2.1
1	A	248	VAL	2.1
1	F	129	GLN	2.1
1	D	180	CYS	2.1
1	A	52	MET	2.1
1	C	452	LEU	2.1
1	C	274	VAL	2.1
1	C	67	GLN	2.1
1	D	67	GLN	2.1
1	D	140	GLN	2.1
1	F	434	ILE	2.1
1	D	68	TYR	2.1
1	D	407	LEU	2.1
1	D	409	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	131	ALA	2.1
1	C	48	ALA	2.1
1	D	302	ASP	2.1
1	E	451	GLU	2.1
1	A	274	VAL	2.1
1	F	130	THR	2.1
1	C	202	GLN	2.1
1	E	288	TRP	2.0
1	A	292	LYS	2.0
1	C	426	GLU	2.0
1	D	57	LEU	2.0
1	D	123	TYR	2.0
1	E	132	ASP	2.0
1	B	91	VAL	2.0
1	C	248	VAL	2.0
1	E	435	GLY	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	MAL	C	3	23/23	0.81	0.24	7.02	76,78,79,79	0
3	NAG	A	1	14/15	0.84	0.21	3.19	50,54,56,57	0
2	MAL	B	2	23/23	0.72	0.23	1.77	71,73,74,76	0
3	NAG	B	3	14/15	0.88	0.16	1.65	42,45,48,50	0
3	NAG	F	11	14/15	0.38	0.52	1.25	70,74,76,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	MAL	B	1	23/23	0.85	0.13	0.47	63,64,64,65	0
3	NAG	D	8	14/15	0.90	0.13	-0.34	32,36,42,45	0
4	CL	E	5	1/1	0.99	0.04	-1.09	31,31,31,31	0
4	CL	C	464	1/1	0.99	0.06	-1.42	24,24,24,24	0
4	CL	B	464	1/1	0.97	0.05	-1.67	29,29,29,29	0
4	CL	A	464	1/1	1.00	0.06	-1.82	26,26,26,26	0
4	CL	F	6	1/1	0.99	0.05	-2.45	28,28,28,28	0
4	CL	D	4	1/1	0.97	0.06	-3.30	31,31,31,31	0
3	NAG	E	9	14/15	0.80	0.17	-	53,57,59,61	0
3	NAG	B	4	14/15	0.80	0.25	-	52,55,59,61	0
3	NAG	A	2	14/15	0.79	0.18	-	44,46,50,51	0
3	NAG	C	5	14/15	0.80	0.31	-	61,66,68,69	0
3	NAG	C	6	14/15	0.68	0.31	-	65,71,73,73	0
3	NAG	E	10	14/15	0.63	0.44	-	61,67,69,70	0
3	NAG	D	7	14/15	0.61	0.54	-	69,73,74,75	0
3	NAG	F	12	14/15	0.32	0.53	-	67,72,74,74	0

6.5 Other polymers (i)

There are no such residues in this entry.