Full wwPDB X-ray Structure Validation Report

Sep 7, 2023 – 02:05 AM EDT

PDB ID	:	4G6B
Title	:	Three dimensional structure analysis of the type II citrate synthase from e.coli
Authors	:	Nguyen, N.T.; Maurus, R.; Stokell, D.J.; Ayed, A.; Duckworth, H.W.; Brayer, G.D.
Deposited on	:	2012-07-18
Resolution	:	2.20 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 (i) 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 (i)) were used in the production of this report:

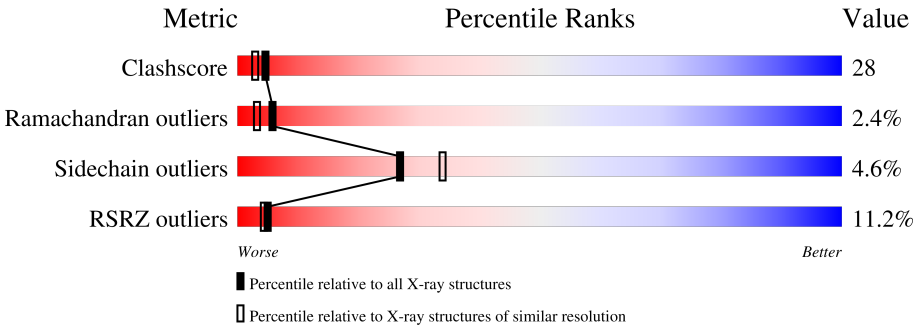
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.20 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	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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	426	12% 65% 30%
1	B	426	10% 62% 33% 5%

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	SO4	B	2001	-	X	-	-
2	SO4	B	2003	-	X	-	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7548 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.

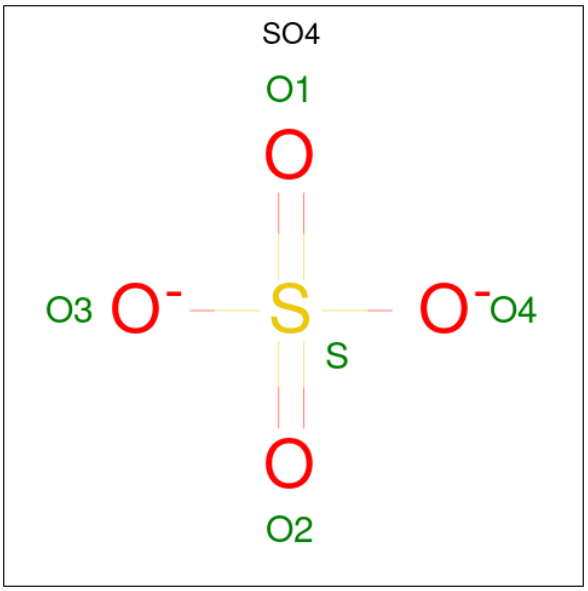
- Molecule 1 is a protein called Citrate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	426	Total	C	N	O	S	0	0	0
			3362	2131	578	628	25			
1	B	426	Total	C	N	O	S	0	0	0
			3362	2131	578	628	25			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	10	ASP	ASN	SEE REMARK 999	UNP P0ABH7
B	10	ASP	ASN	SEE REMARK 999	UNP P0ABH7

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0

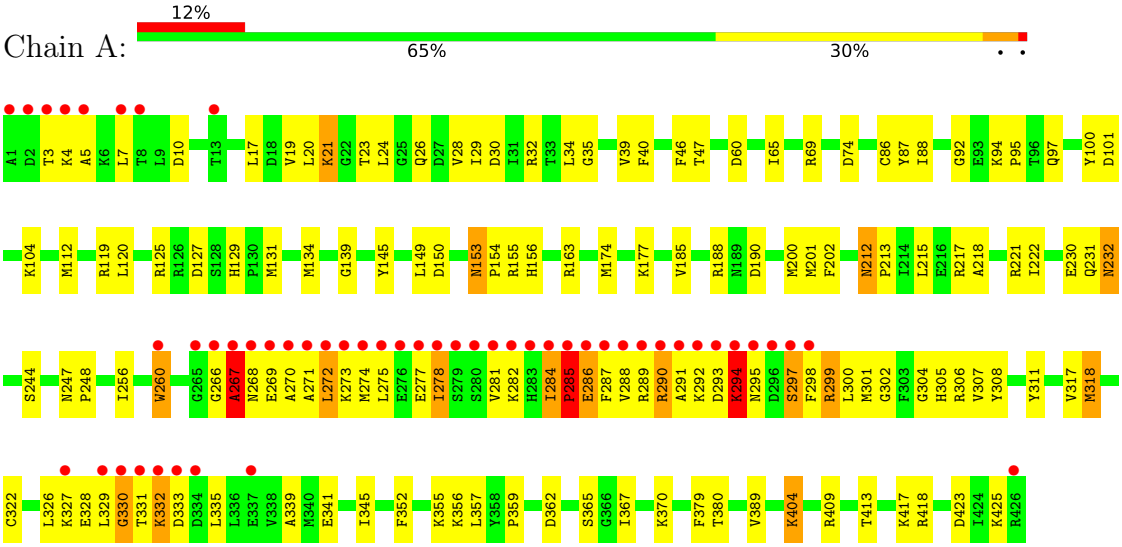
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	386	Total O 386 386	0	0
3	B	408	Total O 408 408	0	0

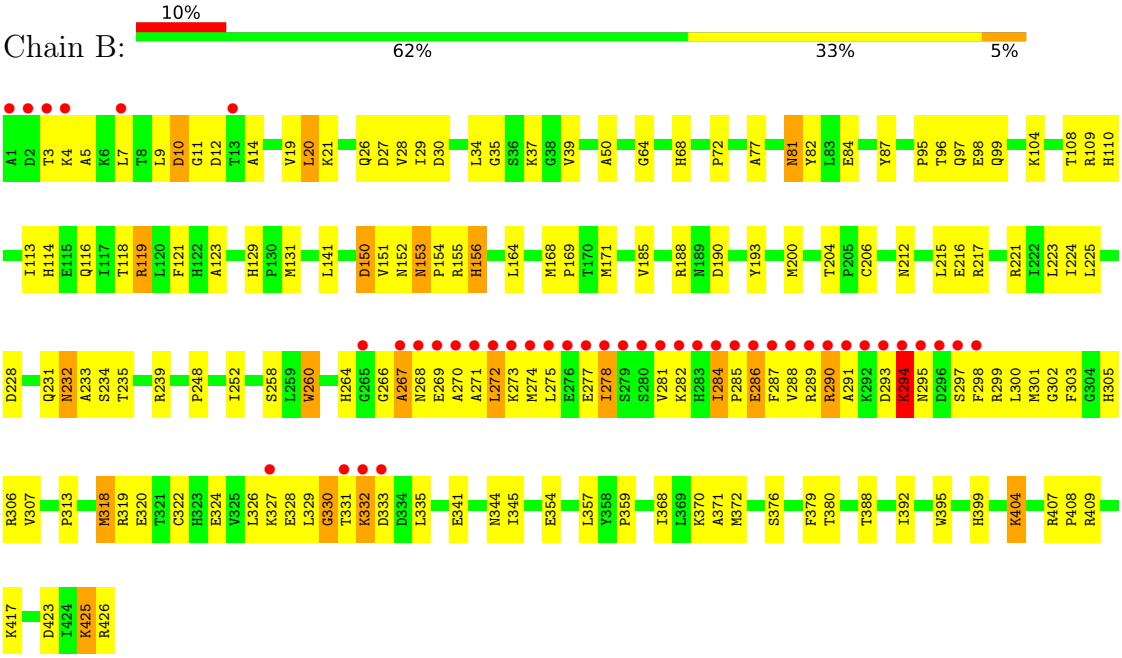
3 Residue-property plots (i)

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: Citrate synthase



• Molecule 1: Citrate synthase



4 Data and refinement statistics (i)

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α, β, γ	165.38Å 165.38Å 155.32Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	10.00 – 2.20 43.88 – 2.20	Depositor EDS
% Data completeness (in resolution range)	100.0 (10.00-2.20) 51.1 (43.88-2.20)	Depositor EDS
R_{merge}	0.93	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	10.42 (at 2.20Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.178 , 0.226 0.194 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	25.6	Xtriage
Anisotropy	0.103	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 81.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.35$	Xtriage
Estimated twinning fraction	0.499 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	7548	wwPDB-VP
Average B, all atoms (Å^2)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.35% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.39	0/3439	0.65	4/4648 (0.1%)
1	B	0.39	0/3439	0.64	2/4648 (0.0%)
All	All	0.39	0/6878	0.64	6/9296 (0.1%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	295	ASN	N-CA-C	-6.26	94.08	111.00
1	B	295	ASN	N-CA-C	-5.91	95.04	111.00
1	A	267	ALA	N-CA-C	-5.48	96.19	111.00
1	A	10	ASP	CB-CG-OD2	5.24	123.01	118.30
1	B	10	ASP	CB-CG-OD2	5.20	122.98	118.30
1	A	202	PHE	N-CA-C	5.10	124.78	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	3362	0	3311	188	0
1	B	3362	0	3311	209	0
2	A	15	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	15	0	0	1	0
3	A	386	0	0	21	0
3	B	408	0	0	18	0
All	All	7548	0	6622	377	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 28.

All (377) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:21:LYS:HE2	1:A:21:LYS:H	1.09	1.10
1:A:285:PRO:HB3	3:A:849:HOH:O	1.54	1.06
1:B:287:PHE:HA	1:B:291:ALA:HB3	1.37	1.05
1:A:269:GLU:HA	1:A:272:LEU:HB2	1.38	1.04
1:A:287:PHE:HA	1:A:291:ALA:HB3	1.40	1.03
1:B:269:GLU:HA	1:B:272:LEU:HB2	1.41	1.03
1:A:281:VAL:HG23	1:A:288:VAL:HG23	1.45	0.98
1:B:281:VAL:HG23	1:B:288:VAL:HG23	1.46	0.98
1:B:274:MET:HG3	1:B:293:ASP:HA	1.45	0.98
1:A:274:MET:HG3	1:A:293:ASP:HA	1.48	0.95
1:A:352:PHE:HA	1:A:357:LEU:HD23	1.51	0.92
1:B:294:LYS:HE2	1:B:357:LEU:HD13	1.51	0.91
1:A:275:LEU:HD22	3:A:824:HOH:O	1.76	0.86
1:B:290:ARG:HA	3:B:2332:HOH:O	1.74	0.86
1:B:114:HIS:HD2	1:B:116:GLN:H	1.21	0.86
1:B:275:LEU:HD11	3:B:2487:HOH:O	1.76	0.83
1:A:21:LYS:H	1:A:21:LYS:CE	1.91	0.83
1:B:204:THR:HG22	1:B:206:CYS:H	1.44	0.83
1:B:129:HIS:HD2	1:B:131:MET:H	1.27	0.81
1:B:81:ASN:HD22	1:B:81:ASN:C	1.84	0.80
1:B:7:LEU:HD21	1:B:29:ILE:HG23	1.64	0.80
1:A:305:HIS:HD2	1:A:307:VAL:H	1.31	0.79
1:B:81:ASN:HD21	1:B:84:GLU:H	1.31	0.79
1:B:20:LEU:HD21	1:B:30:ASP:HB2	1.66	0.78
1:B:81:ASN:ND2	1:B:84:GLU:H	1.80	0.77
1:A:21:LYS:HE2	1:A:21:LYS:N	1.93	0.77
1:B:10:ASP:OD1	1:B:14:ALA:HA	1.84	0.77
1:B:217:ARG:HG3	3:B:2416:HOH:O	1.85	0.77
1:A:355:LYS:HB2	1:A:357:LEU:HD21	1.66	0.77
1:A:294:LYS:HZ1	1:A:298:PHE:H	1.33	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:150:ASP:OD2	1:B:267:ALA:HA	1.85	0.76
1:A:282:LYS:HA	1:A:288:VAL:HG21	1.68	0.76
1:B:7:LEU:HD22	1:B:29:ILE:HG12	1.69	0.75
1:A:150:ASP:H	1:A:156:HIS:HD2	1.35	0.75
1:A:281:VAL:HG23	1:A:288:VAL:CG2	2.17	0.73
1:A:131:MET:HE2	1:A:260:TRP:HB3	1.71	0.73
1:B:129:HIS:CD2	1:B:131:MET:H	2.05	0.73
1:A:7:LEU:HD21	1:A:29:ILE:HG12	1.71	0.72
1:A:266:GLY:C	1:A:270:ALA:HB2	2.10	0.72
1:B:287:PHE:HA	1:B:291:ALA:CB	2.16	0.72
1:A:287:PHE:HA	1:A:291:ALA:CB	2.17	0.72
1:B:272:LEU:HA	1:B:275:LEU:HG	1.72	0.71
1:B:294:LYS:HZ1	1:B:298:PHE:H	1.36	0.71
1:B:305:HIS:HD2	1:B:307:VAL:H	1.38	0.71
1:A:30:ASP:OD1	1:A:32:ARG:HD3	1.90	0.71
1:B:294:LYS:NZ	1:B:298:PHE:H	1.88	0.71
1:A:294:LYS:NZ	1:A:298:PHE:H	1.88	0.71
1:A:281:VAL:O	1:A:288:VAL:HG23	1.91	0.70
1:A:7:LEU:HD23	1:A:19:VAL:HG22	1.72	0.70
1:B:20:LEU:H	1:B:20:LEU:HD22	1.56	0.70
1:B:274:MET:CG	1:B:293:ASP:HA	2.21	0.70
1:A:275:LEU:HA	1:A:289:ARG:HE	1.55	0.70
1:B:275:LEU:CD2	1:B:289:ARG:HE	2.05	0.70
1:B:284:ILE:HD12	1:B:287:PHE:H	1.56	0.69
1:A:284:ILE:HD12	1:A:287:PHE:H	1.56	0.69
1:A:335:LEU:HD23	1:A:335:LEU:H	1.58	0.69
1:A:275:LEU:HA	1:A:289:ARG:NE	2.08	0.69
1:B:335:LEU:HD23	1:B:335:LEU:H	1.59	0.68
1:B:151:VAL:HB	1:B:399:HIS:CE1	2.28	0.68
1:A:272:LEU:HA	1:A:275:LEU:HG	1.76	0.68
1:B:290:ARG:HG3	3:B:2332:HOH:O	1.94	0.68
1:A:327:LYS:HD3	3:A:753:HOH:O	1.94	0.67
1:A:278:ILE:HG12	1:A:288:VAL:HG13	1.77	0.67
1:A:272:LEU:HA	1:A:275:LEU:CD1	2.24	0.67
1:A:274:MET:CG	1:A:293:ASP:HA	2.25	0.67
1:B:212:ASN:HB3	1:B:215:LEU:HG	1.77	0.67
1:B:275:LEU:HD22	1:B:289:ARG:HE	1.59	0.67
1:B:267:ALA:N	1:B:270:ALA:HB2	2.10	0.67
1:A:217:ARG:HD3	1:A:221:ARG:NH1	2.10	0.66
1:B:164:LEU:O	1:B:168:MET:HG2	1.94	0.66
1:B:300:LEU:O	1:B:300:LEU:HD23	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:326:LEU:HG	1:A:333:ASP:CG	2.15	0.66
1:B:275:LEU:HD13	1:B:289:ARG:HH11	1.59	0.66
1:A:274:MET:O	1:A:289:ARG:HG3	1.95	0.66
1:A:129:HIS:HD2	1:A:131:MET:H	1.43	0.66
1:B:272:LEU:N	1:B:272:LEU:HD12	2.12	0.65
1:B:326:LEU:HG	1:B:333:ASP:CG	2.17	0.64
1:B:274:MET:O	1:B:289:ARG:HG3	1.97	0.63
1:B:281:VAL:HG21	3:B:2191:HOH:O	1.98	0.63
1:B:344:ASN:HB2	3:B:2285:HOH:O	1.98	0.63
1:A:215:LEU:HD11	1:A:329:LEU:HD21	1.81	0.63
1:B:150:ASP:H	1:B:156:HIS:HD2	1.46	0.63
1:A:299:ARG:HB2	1:A:304:GLY:O	1.99	0.63
1:A:272:LEU:HD12	1:A:272:LEU:N	2.14	0.63
1:A:413:THR:HG22	1:A:413:THR:O	1.97	0.63
1:A:300:LEU:HD23	1:A:300:LEU:O	1.99	0.62
1:A:272:LEU:HA	1:A:275:LEU:CG	2.30	0.61
1:A:404:LYS:HD2	3:A:920:HOH:O	2.00	0.61
1:A:332:LYS:HG3	3:A:851:HOH:O	2.00	0.61
1:B:290:ARG:HH22	1:B:370:LYS:NZ	1.99	0.61
1:B:169:PRO:HG3	1:B:193:TYR:OH	2.01	0.61
1:A:292:LYS:HE2	3:A:696:HOH:O	1.99	0.61
1:A:120:LEU:HD23	1:B:123:ALA:HB3	1.83	0.60
1:B:278:ILE:HD13	1:B:278:ILE:O	2.00	0.60
1:A:278:ILE:HD13	1:A:278:ILE:O	2.00	0.60
1:A:100:TYR:CE1	1:B:426:ARG:HB3	2.37	0.60
1:A:112:MET:HG2	3:A:716:HOH:O	2.00	0.60
1:A:129:HIS:CD2	1:A:131:MET:H	2.20	0.60
1:B:34:LEU:HD22	1:B:39:VAL:HG11	1.83	0.60
1:B:298:PHE:HD2	1:B:301:MET:HE2	1.67	0.60
1:B:96:THR:HG22	1:B:98:GLU:H	1.66	0.60
1:A:3:THR:C	1:A:5:ALA:H	2.06	0.59
1:A:104:LYS:HD3	1:B:426:ARG:NE	2.17	0.59
1:A:212:ASN:HD22	1:A:213:PRO:CD	2.14	0.59
1:B:11:GLY:HA3	3:B:2318:HOH:O	2.02	0.59
1:B:153:ASN:C	1:B:153:ASN:HD22	2.05	0.59
1:B:274:MET:HB2	1:B:293:ASP:CG	2.23	0.59
3:A:617:HOH:O	1:B:264:HIS:HB3	2.03	0.59
1:A:212:ASN:HD22	1:A:213:PRO:HD2	1.67	0.59
1:B:269:GLU:HB2	1:B:273:LYS:CA	2.33	0.59
1:B:284:ILE:CD1	1:B:287:PHE:H	2.16	0.59
1:A:267:ALA:C	1:A:269:GLU:H	2.06	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:275:LEU:HD22	1:B:289:ARG:NE	2.17	0.58
1:A:289:ARG:CZ	3:A:824:HOH:O	2.51	0.58
1:A:269:GLU:HB2	1:A:273:LYS:CA	2.33	0.58
1:A:100:TYR:HE1	1:B:426:ARG:HB3	1.69	0.58
1:B:275:LEU:HA	1:B:289:ARG:NE	2.18	0.58
1:B:34:LEU:HD22	1:B:39:VAL:CG1	2.34	0.58
1:B:425:LYS:HE3	1:B:425:LYS:HA	1.86	0.58
1:B:267:ALA:C	1:B:269:GLU:H	2.07	0.57
1:A:153:ASN:HD22	1:A:153:ASN:C	2.08	0.57
1:B:20:LEU:CD2	1:B:30:ASP:HB2	2.35	0.57
1:B:7:LEU:HD13	1:B:29:ILE:HD13	1.87	0.57
1:A:34:LEU:HB3	1:A:39:VAL:HB	1.87	0.56
1:B:275:LEU:HD22	1:B:289:ARG:HH11	1.69	0.56
1:A:125:ARG:HB3	1:A:127:ASP:OD1	2.05	0.56
1:A:284:ILE:CD1	1:A:287:PHE:H	2.18	0.56
1:B:131:MET:HE2	1:B:260:TRP:HB3	1.86	0.56
1:B:267:ALA:O	1:B:269:GLU:N	2.38	0.56
1:B:114:HIS:CD2	1:B:116:GLN:H	2.13	0.56
1:B:274:MET:HB2	1:B:293:ASP:OD2	2.05	0.56
1:B:4:LYS:HB3	1:B:21:LYS:HD3	1.86	0.56
1:B:284:ILE:HD12	1:B:287:PHE:N	2.21	0.56
1:B:81:ASN:C	1:B:81:ASN:ND2	2.56	0.55
1:A:7:LEU:HD13	1:B:9:LEU:HD11	1.89	0.55
1:B:7:LEU:HD11	1:B:29:ILE:CG2	2.37	0.55
1:B:141:LEU:HD11	1:B:171:MET:HE1	1.88	0.55
1:A:131:MET:CE	1:A:260:TRP:HB3	2.35	0.55
1:A:7:LEU:C	1:A:7:LEU:HD12	2.27	0.55
1:A:284:ILE:HD12	1:A:287:PHE:N	2.22	0.54
1:A:300:LEU:HB2	3:A:968:HOH:O	2.06	0.54
1:B:98:GLU:HG3	1:B:99:GLN:N	2.22	0.54
1:A:149:LEU:HD22	1:A:247:ASN:HB2	1.90	0.54
1:B:68:HIS:CE1	1:B:228:ASP:HB3	2.43	0.54
1:A:94:LYS:HG2	3:A:773:HOH:O	2.08	0.54
1:A:273:LYS:NZ	1:A:273:LYS:HB3	2.23	0.54
1:A:404:LYS:CD	3:A:920:HOH:O	2.56	0.54
1:A:274:MET:HB2	1:A:293:ASP:CG	2.28	0.54
1:B:113:ILE:HD11	1:B:118:THR:OG1	2.08	0.54
1:B:425:LYS:HE3	1:B:425:LYS:CA	2.38	0.54
1:A:277:GLU:O	1:A:277:GLU:HG2	2.08	0.53
1:B:232:ASN:ND2	1:B:235:THR:H	2.05	0.53
1:B:277:GLU:HG2	1:B:277:GLU:O	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:275:LEU:HD22	1:B:289:ARG:NH1	2.23	0.53
1:B:131:MET:HE2	1:B:380:THR:HG22	1.91	0.53
1:B:320:GLU:O	1:B:324:GLU:HG3	2.09	0.53
1:A:274:MET:HB2	1:A:293:ASP:OD2	2.08	0.53
1:A:7:LEU:HD23	1:A:19:VAL:CG2	2.39	0.52
1:A:150:ASP:H	1:A:156:HIS:CD2	2.20	0.52
1:B:284:ILE:HG23	1:B:284:ILE:O	2.10	0.52
1:A:404:LYS:HE3	3:A:694:HOH:O	2.08	0.52
1:A:355:LYS:HB2	1:A:357:LEU:CD2	2.38	0.52
1:A:404:LYS:HD3	1:A:404:LYS:N	2.24	0.52
1:B:273:LYS:NZ	1:B:273:LYS:HB3	2.25	0.52
1:B:20:LEU:HD23	1:B:28:VAL:HG23	1.92	0.52
1:A:7:LEU:HD11	1:A:17:LEU:HB2	1.91	0.52
1:A:145:TYR:HB3	1:A:163:ARG:NH2	2.24	0.52
1:A:47:THR:HG23	1:B:409:ARG:HH11	1.75	0.52
1:A:328:GLU:C	1:A:330:GLY:H	2.12	0.51
1:B:204:THR:HG22	1:B:206:CYS:N	2.21	0.51
1:B:305:HIS:CD2	1:B:307:VAL:H	2.23	0.51
1:A:417:LYS:HD3	1:A:417:LYS:C	2.31	0.51
1:B:82:TYR:CD1	1:B:223:LEU:HB3	2.45	0.51
1:A:272:LEU:HA	1:A:275:LEU:HD12	1.91	0.51
1:A:404:LYS:HD3	1:A:404:LYS:H	1.76	0.51
1:A:404:LYS:HG2	1:A:404:LYS:O	2.11	0.51
1:B:96:THR:CG2	1:B:98:GLU:HG2	2.41	0.51
1:B:328:GLU:C	1:B:330:GLY:H	2.12	0.51
1:B:267:ALA:C	1:B:269:GLU:N	2.62	0.51
1:B:272:LEU:HA	1:B:275:LEU:CG	2.40	0.51
1:A:267:ALA:C	1:A:269:GLU:N	2.63	0.51
1:A:275:LEU:CD2	1:A:289:ARG:HE	2.23	0.51
1:B:275:LEU:HA	1:B:289:ARG:HE	1.75	0.51
1:A:7:LEU:CD1	1:A:17:LEU:HB2	2.41	0.51
1:B:248:PRO:HG3	1:B:395:TRP:CZ2	2.46	0.51
1:A:292:LYS:NZ	3:A:696:HOH:O	2.45	0.50
1:A:326:LEU:HG	1:A:333:ASP:OD1	2.12	0.50
1:B:318:MET:CE	1:B:318:MET:HA	2.42	0.50
1:A:97:GLN:OE1	1:B:425:LYS:N	2.44	0.50
1:A:362:ASP:HA	1:A:365:SER:HB2	1.93	0.50
1:B:4:LYS:HD2	1:B:21:LYS:CD	2.41	0.50
1:B:3:THR:O	1:B:19:VAL:HG11	2.12	0.50
1:B:404:LYS:O	1:B:404:LYS:HG2	2.12	0.50
1:A:88:ILE:HG12	1:A:94:LYS:HA	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:288:VAL:HG13	1:A:289:ARG:N	2.27	0.50
1:B:303:PHE:HB3	1:B:357:LEU:HB3	1.94	0.50
1:A:284:ILE:HG23	1:A:284:ILE:O	2.12	0.50
1:B:284:ILE:HD13	1:B:284:ILE:C	2.32	0.50
1:B:21:LYS:HG2	1:B:27:ASP:OD1	2.12	0.49
1:B:64:GLY:O	1:B:313:PRO:HB3	2.12	0.49
1:B:231:GLN:HE22	1:B:239:ARG:NE	2.10	0.49
1:A:278:ILE:HG12	1:A:288:VAL:CG1	2.41	0.49
1:A:153:ASN:ND2	1:A:155:ARG:H	2.09	0.49
1:B:289:ARG:O	1:B:291:ALA:N	2.41	0.49
1:B:404:LYS:H	1:B:404:LYS:HD3	1.77	0.49
1:A:188:ARG:NH1	1:A:190:ASP:OD2	2.44	0.49
1:B:404:LYS:HD3	1:B:404:LYS:N	2.27	0.49
1:A:290:ARG:HH22	1:A:370:LYS:NZ	2.09	0.49
1:B:368:ILE:O	1:B:372:MET:HG3	2.12	0.49
1:A:7:LEU:HD21	1:A:29:ILE:CG1	2.42	0.49
1:A:282:LYS:CA	1:A:288:VAL:HG21	2.40	0.49
1:B:153:ASN:O	1:B:156:HIS:HB2	2.13	0.49
1:B:268:ASN:O	1:B:272:LEU:HD22	2.12	0.49
1:A:284:ILE:C	1:A:284:ILE:HD13	2.32	0.48
1:A:318:MET:HA	1:A:318:MET:CE	2.43	0.48
1:A:418:ARG:O	1:B:72:PRO:HD3	2.13	0.48
1:B:164:LEU:HD13	1:B:252:ILE:HG13	1.94	0.48
1:B:131:MET:HE2	1:B:380:THR:CG2	2.44	0.48
1:B:287:PHE:CA	1:B:291:ALA:HB3	2.27	0.48
1:B:109:ARG:NH2	3:B:2479:HOH:O	2.46	0.48
1:B:269:GLU:HB2	1:B:273:LYS:HA	1.96	0.48
1:B:131:MET:CE	1:B:380:THR:HG22	2.43	0.48
1:B:275:LEU:HB3	1:B:289:ARG:NH1	2.28	0.48
1:B:326:LEU:HG	1:B:333:ASP:OD1	2.14	0.48
1:A:185:VAL:HB	1:A:200:MET:HA	1.96	0.48
1:A:269:GLU:HB2	1:A:273:LYS:HA	1.96	0.48
1:A:423:ASP:HB3	3:B:2319:HOH:O	2.14	0.48
1:A:425:LYS:H	1:B:97:GLN:HE22	1.62	0.48
1:A:87:TYR:CD1	1:A:95:PRO:HB3	2.49	0.47
1:A:120:LEU:HD23	1:B:123:ALA:CB	2.43	0.47
1:A:217:ARG:HH21	1:A:221:ARG:NH1	2.12	0.47
1:A:230:GLU:CG	1:A:231:GLN:H	2.27	0.47
1:A:341:GLU:O	1:A:345:ILE:HG13	2.14	0.47
1:A:153:ASN:HD22	1:A:154:PRO:N	2.13	0.47
1:A:217:ARG:HD3	1:A:221:ARG:HH11	1.76	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:232:ASN:C	1:A:232:ASN:HD22	2.18	0.47
1:B:26:GLN:NE2	3:B:2437:HOH:O	2.46	0.47
1:B:277:GLU:O	1:B:281:VAL:HG22	2.15	0.47
1:A:409:ARG:HB2	1:B:50:ALA:HA	1.96	0.47
1:A:281:VAL:C	1:A:288:VAL:HG23	2.34	0.47
1:B:278:ILE:HA	1:B:288:VAL:HG22	1.95	0.47
1:A:7:LEU:CD2	1:A:29:ILE:HG12	2.43	0.47
1:B:153:ASN:C	1:B:153:ASN:ND2	2.67	0.47
1:B:332:LYS:O	1:B:335:LEU:HD21	2.13	0.47
1:B:269:GLU:O	1:B:273:LYS:HB2	2.14	0.47
1:B:290:ARG:NH1	3:B:2492:HOH:O	2.43	0.47
1:B:77:ALA:HB2	1:B:225:LEU:HD21	1.96	0.47
1:B:221:ARG:O	1:B:225:LEU:HG	2.14	0.47
1:B:275:LEU:HB2	3:B:2260:HOH:O	2.14	0.47
1:B:318:MET:O	1:B:322:CYS:HB2	2.14	0.47
1:A:269:GLU:O	1:A:273:LYS:HB2	2.14	0.47
1:B:271:ALA:H	1:B:272:LEU:HD12	1.79	0.47
1:A:267:ALA:N	1:A:270:ALA:HB2	2.29	0.47
1:A:298:PHE:HD2	1:A:301:MET:HE2	1.79	0.47
1:B:87:TYR:CD1	1:B:95:PRO:HB3	2.51	0.47
1:A:174:MET:HG3	3:A:875:HOH:O	2.15	0.46
1:B:77:ALA:HA	1:B:224:ILE:HG21	1.98	0.46
1:B:118:THR:O	1:B:121:PHE:HB2	2.15	0.46
1:B:248:PRO:HG3	1:B:395:TRP:CH2	2.50	0.46
1:B:341:GLU:O	1:B:345:ILE:HG13	2.15	0.46
1:B:322:CYS:O	1:B:326:LEU:HD13	2.15	0.46
1:A:277:GLU:O	1:A:281:VAL:HG22	2.16	0.46
1:A:292:LYS:CE	3:A:696:HOH:O	2.59	0.46
1:B:7:LEU:CD2	1:B:29:ILE:HG12	2.40	0.46
1:A:357:LEU:N	1:A:357:LEU:HD22	2.31	0.46
1:A:308:TYR:HB3	1:A:311:TYR:O	2.14	0.46
1:A:287:PHE:CA	1:A:291:ALA:HB3	2.29	0.46
1:B:7:LEU:HD11	1:B:29:ILE:HG21	1.97	0.45
1:A:305:HIS:CD2	1:A:307:VAL:H	2.21	0.45
1:B:104:LYS:O	1:B:108:THR:HG23	2.16	0.45
1:B:188:ARG:HB3	1:B:190:ASP:OD1	2.16	0.45
1:B:275:LEU:CD1	1:B:289:ARG:HH11	2.28	0.45
1:A:7:LEU:HB2	1:B:10:ASP:O	2.16	0.45
1:B:7:LEU:HD11	1:B:29:ILE:HG23	1.98	0.45
1:B:96:THR:HG21	1:B:98:GLU:HG2	1.99	0.45
1:B:110:HIS:HB2	3:B:2483:HOH:O	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:376:SER:HA	1:B:379:PHE:CZ	2.52	0.45
1:A:339:ALA:HB1	1:A:367:ILE:HD13	1.98	0.45
1:B:289:ARG:C	1:B:291:ALA:H	2.19	0.45
1:A:86:CYS:HA	1:A:389:VAL:HG21	1.98	0.45
1:A:212:ASN:HD22	1:A:213:PRO:N	2.14	0.45
1:B:282:LYS:HD2	1:B:282:LYS:O	2.16	0.45
1:B:289:ARG:CZ	3:B:2492:HOH:O	2.63	0.45
1:B:305:HIS:HE1	2:B:2003:SO4:O4	2.00	0.45
1:B:289:ARG:HG2	1:B:290:ARG:N	2.32	0.44
1:B:327:LYS:O	1:B:327:LYS:HG2	2.17	0.44
1:A:275:LEU:HD22	1:A:289:ARG:HH11	1.82	0.44
1:A:404:LYS:O	1:A:404:LYS:CG	2.64	0.44
1:A:134:MET:HG2	1:A:256:ILE:HG21	2.00	0.44
1:B:119:ARG:HA	1:B:119:ARG:HD2	1.85	0.44
1:A:282:LYS:HA	1:A:288:VAL:CG2	2.44	0.44
1:B:266:GLY:C	1:B:270:ALA:HB2	2.37	0.44
1:B:286:GLU:C	1:B:288:VAL:H	2.20	0.44
1:B:335:LEU:HD23	1:B:335:LEU:N	2.31	0.44
1:B:275:LEU:HD22	1:B:289:ARG:CZ	2.48	0.44
1:B:319:ARG:HD3	3:B:2152:HOH:O	2.17	0.44
1:B:212:ASN:HB3	1:B:215:LEU:CG	2.47	0.44
1:A:177:LYS:HE2	1:A:201:MET:O	2.16	0.43
1:A:268:ASN:O	1:A:272:LEU:HD22	2.17	0.43
1:A:275:LEU:HD22	1:A:289:ARG:HE	1.82	0.43
1:A:356:LYS:HE3	3:A:796:HOH:O	2.17	0.43
1:A:370:LYS:HG3	1:A:379:PHE:HZ	1.83	0.43
1:B:234:SER:HA	1:B:258:SER:OG	2.18	0.43
1:B:272:LEU:N	1:B:272:LEU:CD1	2.81	0.43
1:A:20:LEU:HB2	1:A:28:VAL:CG2	2.49	0.43
1:A:335:LEU:HD23	1:A:335:LEU:N	2.31	0.43
1:B:306:ARG:C	1:B:306:ARG:HD2	2.39	0.43
1:B:278:ILE:O	1:B:278:ILE:CD1	2.66	0.43
1:A:212:ASN:ND2	1:A:213:PRO:HD2	2.34	0.43
1:A:287:PHE:O	1:A:292:LYS:HB2	2.19	0.43
1:B:329:LEU:HD13	1:B:371:ALA:O	2.17	0.43
1:A:289:ARG:HG2	1:A:290:ARG:N	2.33	0.43
1:A:302:GLY:O	1:A:359:PRO:HA	2.19	0.43
1:B:152:ASN:O	1:B:154:PRO:HD3	2.18	0.43
1:B:168:MET:HB2	1:B:169:PRO:HD3	2.01	0.43
1:B:290:ARG:NE	3:B:2492:HOH:O	2.48	0.43
1:A:289:ARG:NH2	3:A:912:HOH:O	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:425:LYS:H	1:B:97:GLN:NE2	2.16	0.43
1:A:271:ALA:H	1:A:272:LEU:HD12	1.83	0.43
1:A:286:GLU:C	1:A:288:VAL:H	2.21	0.43
1:B:151:VAL:HB	1:B:399:HIS:NE2	2.33	0.43
1:B:404:LYS:O	1:B:404:LYS:CG	2.66	0.43
1:B:423:ASP:HA	3:B:2273:HOH:O	2.19	0.43
1:A:101:ASP:HA	1:B:426:ARG:HH21	1.84	0.42
1:A:278:ILE:O	1:A:278:ILE:CD1	2.67	0.42
1:B:274:MET:CB	1:B:293:ASP:HA	2.48	0.42
1:B:35:GLY:C	1:B:37:LYS:H	2.22	0.42
1:B:151:VAL:HG11	3:B:2256:HOH:O	2.19	0.42
1:A:74:ASP:OD1	1:A:317:VAL:HG23	2.20	0.42
1:A:149:LEU:HD22	1:A:247:ASN:CB	2.50	0.42
1:B:278:ILE:O	1:B:278:ILE:HG23	2.20	0.42
1:A:30:ASP:OD2	1:A:32:ARG:NH2	2.53	0.42
1:A:104:LYS:NZ	1:B:426:ARG:HG2	2.34	0.42
1:B:153:ASN:ND2	1:B:155:ARG:H	2.17	0.42
1:A:23:THR:O	1:A:24:LEU:HD23	2.19	0.42
1:A:326:LEU:HG	1:A:333:ASP:OD2	2.19	0.42
1:A:417:LYS:NZ	3:A:797:HOH:O	2.48	0.42
1:A:131:MET:HE2	1:A:380:THR:CG2	2.49	0.42
1:B:150:ASP:OD2	1:B:150:ASP:N	2.52	0.42
1:A:150:ASP:HB3	1:A:156:HIS:CD2	2.55	0.41
1:B:298:PHE:CD2	1:B:301:MET:HE2	2.51	0.41
1:B:19:VAL:HA	1:B:28:VAL:O	2.20	0.41
1:B:275:LEU:HD13	1:B:289:ARG:NH1	2.30	0.41
1:A:35:GLY:HA2	1:A:40:PHE:CE2	2.55	0.41
1:A:139:GLY:HA3	3:A:642:HOH:O	2.20	0.41
1:B:302:GLY:O	1:B:359:PRO:HA	2.20	0.41
1:A:294:LYS:HZ2	1:A:297:SER:HA	1.85	0.41
1:B:284:ILE:HD12	1:B:287:PHE:HB2	2.02	0.41
1:A:69:ARG:CD	1:A:92:GLY:HA2	2.51	0.41
1:B:4:LYS:HD2	1:B:21:LYS:HD3	2.03	0.41
1:A:244:SER:HB3	1:B:233:ALA:HB1	2.01	0.41
1:A:272:LEU:N	1:A:272:LEU:CD1	2.83	0.41
1:A:278:ILE:O	1:A:278:ILE:HG23	2.21	0.41
1:B:7:LEU:CD2	1:B:29:ILE:HG23	2.42	0.41
1:B:185:VAL:HB	1:B:200:MET:HA	2.02	0.41
3:A:793:HOH:O	1:B:39:VAL:HA	2.20	0.41
1:A:3:THR:O	1:A:5:ALA:N	2.53	0.41
1:A:46:PHE:O	1:B:408:PRO:HA	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:218:ALA:O	1:A:222:ILE:HG13	2.21	0.41
1:A:275:LEU:HB3	1:A:289:ARG:HH11	1.86	0.41
1:A:282:LYS:HD2	1:A:282:LYS:O	2.20	0.41
1:A:332:LYS:O	1:A:335:LEU:HD21	2.20	0.41
1:A:60:ASP:HB3	1:A:65:ILE:HB	2.03	0.41
1:A:104:LYS:HD3	1:B:426:ARG:CZ	2.51	0.41
1:A:212:ASN:HD22	1:A:212:ASN:C	2.25	0.41
1:A:274:MET:CB	1:A:293:ASP:HA	2.50	0.41
1:A:306:ARG:HD3	1:B:407:ARG:NH1	2.36	0.41
1:B:282:LYS:HA	1:B:288:VAL:HG21	2.02	0.40
1:B:425:LYS:HE3	1:B:425:LYS:C	2.41	0.40
1:B:3:THR:C	1:B:5:ALA:H	2.25	0.40
1:B:20:LEU:O	1:B:27:ASP:HB3	2.21	0.40
1:A:247:ASN:HB2	1:A:248:PRO:HD2	2.02	0.40
1:A:274:MET:SD	1:A:277:GLU:OE2	2.79	0.40
1:B:417:LYS:HD3	1:B:417:LYS:C	2.41	0.40
1:A:322:CYS:O	1:A:326:LEU:HD13	2.21	0.40
1:B:271:ALA:O	1:B:275:LEU:HG	2.21	0.40
1:B:388:THR:O	1:B:392:ILE:HG13	2.22	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	424/426 (100%)	379 (89%)	35 (8%)	10 (2%)	6 3
1	B	424/426 (100%)	379 (89%)	35 (8%)	10 (2%)	6 3
All	All	848/852 (100%)	758 (89%)	70 (8%)	20 (2%)	6 3

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	297	SER
1	A	4	LYS
1	A	267	ALA
1	A	290	ARG
1	A	294	LYS
1	A	331	THR
1	B	267	ALA
1	B	290	ARG
1	B	294	LYS
1	B	331	THR
1	B	332	LYS
1	A	285	PRO
1	A	330	GLY
1	A	332	LYS
1	B	12	ASP
1	B	285	PRO
1	B	286	GLU
1	A	286	GLU
1	B	297	SER
1	B	330	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	361/361 (100%)	346 (96%)	15 (4%)	30	38
1	B	361/361 (100%)	343 (95%)	18 (5%)	24	30
All	All	722/722 (100%)	689 (95%)	33 (5%)	27	34

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	LYS
1	A	26	GLN
1	A	119	ARG
1	A	153	ASN

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Mol	Chain	Res	Type
1	A	212	ASN
1	A	232	ASN
1	A	260	TRP
1	A	272	LEU
1	A	278	ILE
1	A	284	ILE
1	A	285	PRO
1	A	294	LYS
1	A	299	ARG
1	A	318	MET
1	A	404	LYS
1	B	20	LEU
1	B	81	ASN
1	B	119	ARG
1	B	150	ASP
1	B	153	ASN
1	B	156	HIS
1	B	216	GLU
1	B	232	ASN
1	B	260	TRP
1	B	272	LEU
1	B	278	ILE
1	B	284	ILE
1	B	294	LYS
1	B	299	ARG
1	B	318	MET
1	B	354	GLU
1	B	404	LYS
1	B	425	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	99	GLN
1	A	129	HIS
1	A	153	ASN
1	A	156	HIS
1	A	182	GLN
1	A	212	ASN
1	A	231	GLN
1	A	232	ASN
1	A	305	HIS

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Mol	Chain	Res	Type
1	A	323	HIS
1	A	399	HIS
1	B	26	GLN
1	B	81	ASN
1	B	91	ASN
1	B	97	GLN
1	B	110	HIS
1	B	114	HIS
1	B	129	HIS
1	B	152	ASN
1	B	153	ASN
1	B	156	HIS
1	B	231	GLN
1	B	232	ASN
1	B	305	HIS
1	B	399	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

6 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	SO4	A	502	-	4,4,4	0.70	0	6,6,6	0.40	0
2	SO4	B	2002	-	4,4,4	0.67	0	6,6,6	0.30	0
2	SO4	B	2001	-	4,4,4	0.57	0	6,6,6	3.84	4 (66%)
2	SO4	B	2003	-	4,4,4	0.59	0	6,6,6	3.87	4 (66%)
2	SO4	A	501	-	4,4,4	0.61	0	6,6,6	0.35	0
2	SO4	A	503	-	4,4,4	0.68	0	6,6,6	0.43	0

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	2003	SO4	O4-S-O1	-5.76	79.25	109.31
2	B	2001	SO4	O4-S-O1	-5.58	80.20	109.31
2	B	2003	SO4	O4-S-O3	-5.23	86.73	109.06
2	B	2001	SO4	O4-S-O3	-5.13	87.17	109.06
2	B	2001	SO4	O4-S-O2	-4.83	84.09	109.31
2	B	2003	SO4	O4-S-O2	-4.66	84.97	109.31
2	B	2001	SO4	O2-S-O1	2.44	127.49	109.43
2	B	2003	SO4	O2-S-O1	2.36	126.83	109.43

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	2003	SO4	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	426/426 (100%)	0.25	52 (12%)	4	3	15, 27, 140, 182	0
1	B	426/426 (100%)	0.18	43 (10%)	7	6	12, 27, 141, 181	0
All	All	852/852 (100%)	0.22	95 (11%)	5	4	12, 27, 141, 182	0

All (95) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	281	VAL	21.9
1	A	281	VAL	18.0
1	A	278	ILE	15.6
1	A	284	ILE	14.5
1	A	297	SER	14.4
1	A	331	THR	14.1
1	B	280	SER	13.9
1	B	4	LYS	13.7
1	B	274	MET	12.5
1	B	278	ILE	12.1
1	B	1	ALA	12.0
1	A	280	SER	12.0
1	B	297	SER	12.0
1	A	268	ASN	10.9
1	B	331	THR	10.8
1	B	284	ILE	10.8
1	A	282	LYS	10.7
1	B	267	ALA	10.7
1	B	2	ASP	10.2
1	B	288	VAL	10.1
1	A	274	MET	10.0
1	A	1	ALA	9.9
1	A	267	ALA	9.6
1	A	283	HIS	9.5

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Mol	Chain	Res	Type	RSRZ
1	B	283	HIS	9.4
1	A	288	VAL	9.1
1	A	269	GLU	8.9
1	B	269	GLU	8.7
1	A	265	GLY	8.3
1	A	275	LEU	8.1
1	B	282	LYS	8.0
1	A	4	LYS	7.9
1	B	275	LEU	7.7
1	A	279	SER	7.7
1	A	266	GLY	7.6
1	A	290	ARG	7.4
1	A	287	PHE	7.2
1	A	3	THR	6.8
1	B	279	SER	6.6
1	B	290	ARG	6.4
1	B	268	ASN	6.4
1	A	2	ASP	6.3
1	B	3	THR	6.2
1	B	291	ALA	6.2
1	B	287	PHE	6.0
1	A	333	ASP	6.0
1	B	285	PRO	6.0
1	B	293	ASP	5.9
1	B	276	GLU	5.8
1	B	333	ASP	5.8
1	A	293	ASP	5.8
1	A	277	GLU	5.5
1	A	291	ALA	5.5
1	A	332	LYS	5.4
1	A	271	ALA	5.4
1	B	277	GLU	5.3
1	B	273	LYS	5.2
1	A	273	LYS	5.0
1	B	286	GLU	4.8
1	A	285	PRO	4.7
1	B	265	GLY	4.5
1	B	298	PHE	4.5
1	A	286	GLU	4.4
1	A	295	ASN	4.4
1	B	271	ALA	4.0
1	B	332	LYS	3.9

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Mol	Chain	Res	Type	RSRZ
1	B	7	LEU	3.8
1	A	298	PHE	3.6
1	A	330	GLY	3.3
1	B	294	LYS	3.3
1	A	294	LYS	3.2
1	A	7	LEU	3.1
1	B	270	ALA	3.0
1	B	289	ARG	3.0
1	A	270	ALA	2.9
1	A	289	ARG	2.9
1	A	272	LEU	2.8
1	B	272	LEU	2.8
1	A	5	ALA	2.7
1	A	276	GLU	2.7
1	A	329	LEU	2.7
1	A	327	LYS	2.6
1	A	426	ARG	2.6
1	B	295	ASN	2.6
1	A	334	ASP	2.5
1	A	292	LYS	2.4
1	B	292	LYS	2.4
1	A	13	THR	2.4
1	B	13	THR	2.3
1	A	296	ASP	2.2
1	B	327	LYS	2.2
1	A	260	TRP	2.1
1	A	337	GLU	2.1
1	B	296	ASP	2.1
1	A	8	THR	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

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
2	SO4	A	501	5/5	0.99	0.12	22,23,25,27	0
2	SO4	A	502	5/5	0.99	0.10	37,39,42,42	0
2	SO4	A	503	5/5	0.99	0.10	24,25,28,28	0
2	SO4	B	2001	5/5	0.99	0.13	29,31,33,34	0
2	SO4	B	2002	5/5	0.99	0.13	34,36,38,41	0
2	SO4	B	2003	5/5	0.99	0.13	39,39,43,45	0

6.5 Other polymers

There are no such residues in this entry.