Full wwPDB X-ray Structure Validation Report ⓘ

Aug 21, 2020 – 03:22 PM BST

PDB ID	:	1SRQ
Title	:	Crystal Structure of the Rap1GAP catalytic domain
Authors	:	Daumke, O.; Weyand, M.; Chakrabarti, P.P.; Vetter, I.R.; Wittinghofer, A.
Deposited on	:	2004-03-23
Resolution	:	2.90 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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

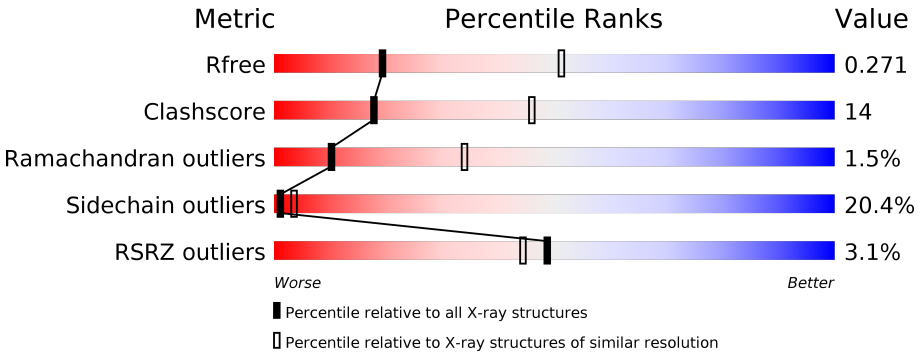
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

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 2.90 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))
R_{free}	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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 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	341	2% 61% 28% 6%
1	B	341	3% 52% 30% 7% 11%
1	C	341	% 58% 27% 9% 5%
1	D	341	3% 12% 5% 81%

2 Entry composition

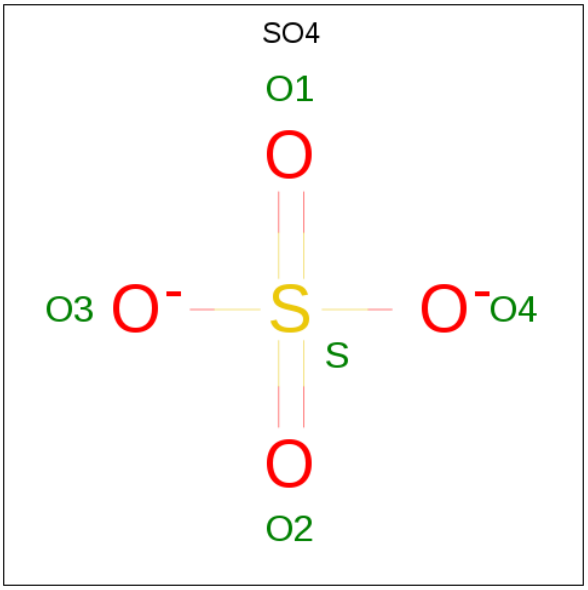
There are 4 unique types of molecules in this entry. The entry contains 8241 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 GTPase-activating protein 1.

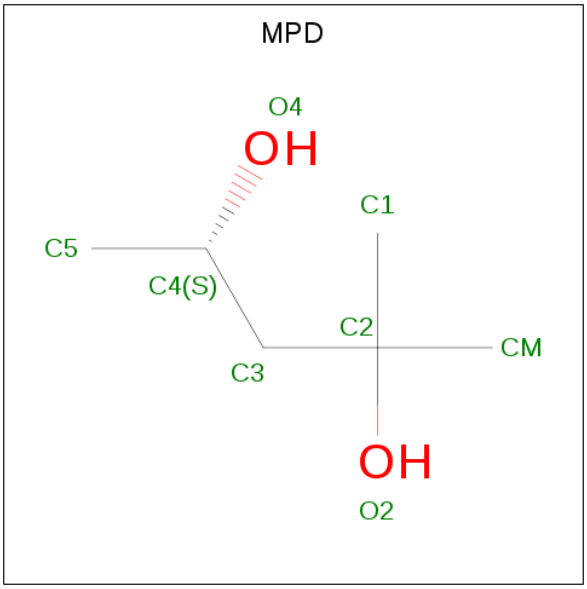
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	330	Total	C	N	O	S	0	0	0
			2650	1710	444	486	10			
1	B	304	Total	C	N	O	S	0	0	0
			2423	1574	406	433	10			
1	C	324	Total	C	N	O	S	0	0	0
			2619	1694	439	476	10			
1	D	66	Total	C	N	O	S	0	0	0
			476	305	80	89	2			

- 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			
2	C	1	Total	O	S		0	0
			5	4	1			

- Molecule 3 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: $C_6H_{14}O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 8 6 2	0	0
3	C	1	Total C O 8 6 2	0	0

- Molecule 4 is water.

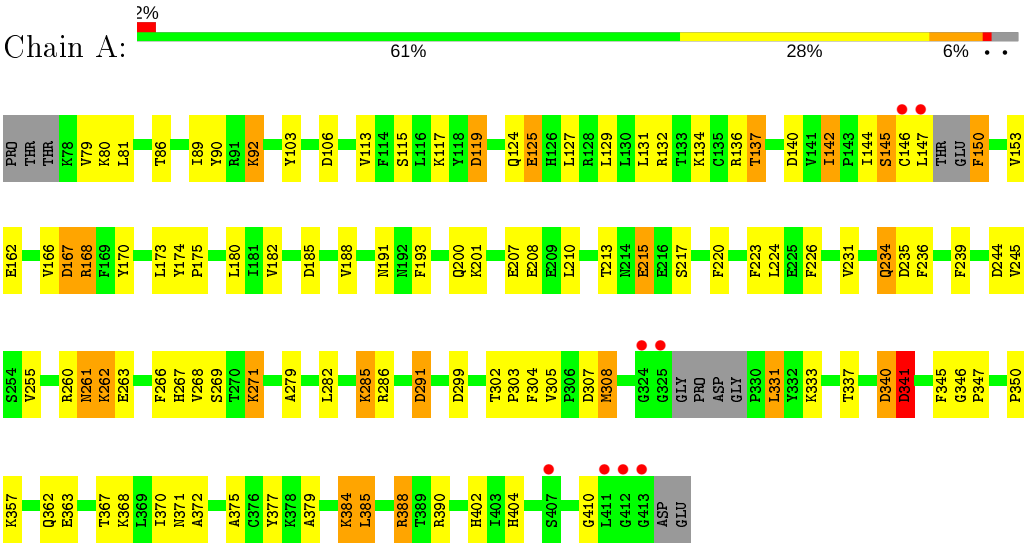
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	15	Total O 15 15	0	0
4	B	6	Total O 6 6	0	0
4	C	25	Total O 25 25	0	0
4	D	1	Total O 1 1	0	0

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.

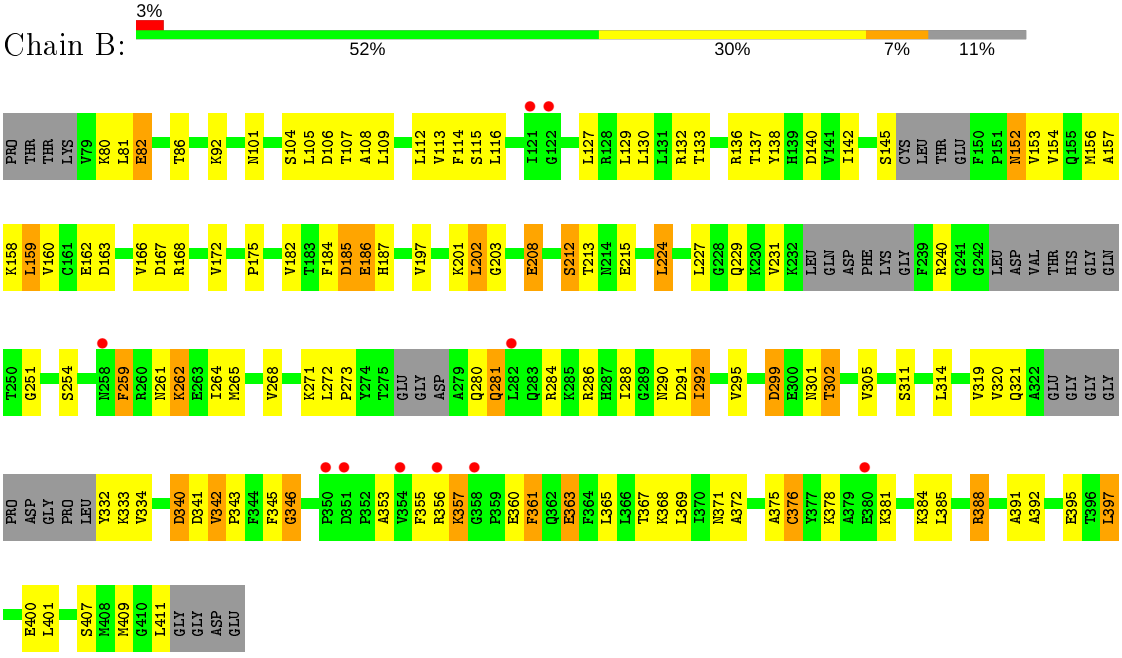
- Molecule 1: GTPase-activating protein 1

Chain A:



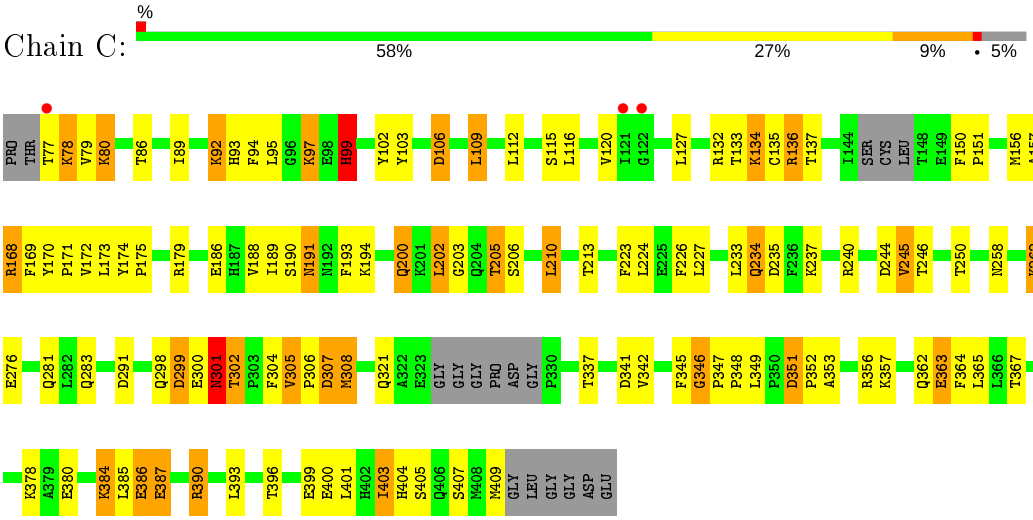
- Molecule 1: GTPase-activating protein 1

Chain B:



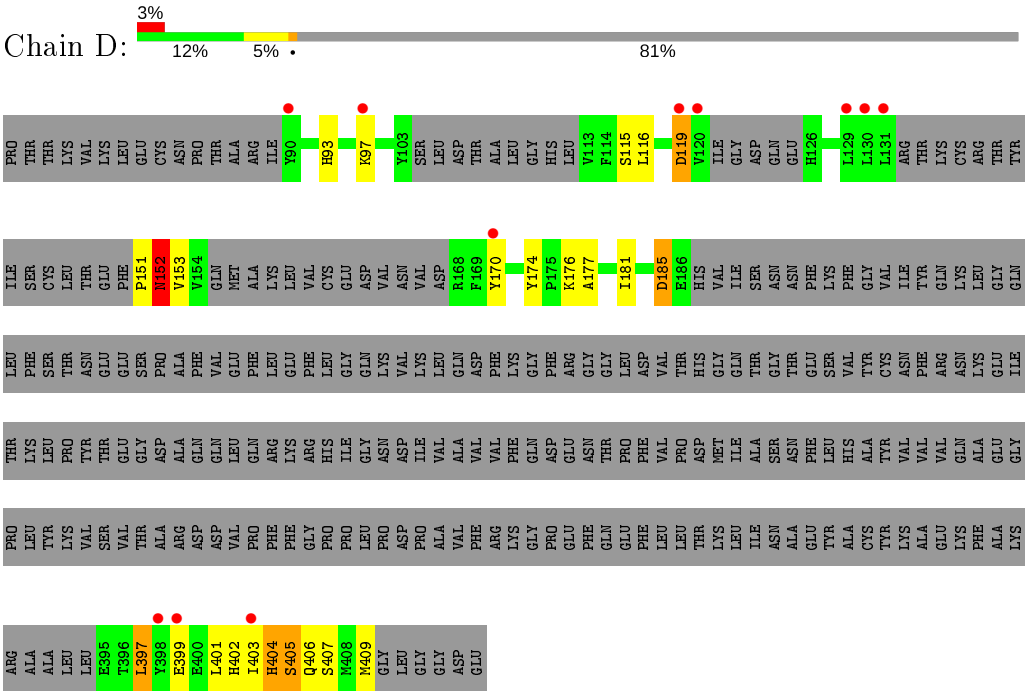
• Molecule 1: GTPase-activating protein 1

Chain C:



• Molecule 1: GTPase-activating protein 1

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	170.70Å 224.50Å 48.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	14.99 – 2.90 14.99 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.4 (14.99-2.90) 99.4 (14.99-2.90)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [1]	3.40 (at 2.91Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.232 , 0.276 0.228 , 0.271	Depositor DCC
R_{free} test set	2103 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	77.4	Xtriage
Anisotropy	0.427	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.26 , 41.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	8241	wwPDB-VP
Average B, all atoms (Å^2)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.00% 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: MPD, 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	0.83	0/2714	1.04	12/3670 (0.3%)
1	B	0.58	0/2481	0.81	2/3357 (0.1%)
1	C	0.77	1/2683 (0.0%)	0.99	9/3630 (0.2%)
1	D	0.48	0/481	0.76	3/649 (0.5%)
All	All	0.73	1/8359 (0.0%)	0.95	26/11306 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	136	ARG	CG-CD	5.12	1.64	1.51

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	351	ASP	CB-CG-OD2	9.12	126.50	118.30
1	C	307	ASP	CB-CG-OD2	6.92	124.53	118.30
1	A	119	ASP	CB-CG-OD2	6.72	124.35	118.30
1	C	291	ASP	CB-CG-OD2	6.64	124.28	118.30
1	A	167	ASP	CB-CG-OD2	6.58	124.22	118.30
1	A	331	LEU	CA-CB-CG	6.56	130.38	115.30
1	A	351	ASP	CB-CG-OD2	6.17	123.86	118.30
1	C	106	ASP	CB-CG-OD2	6.15	123.83	118.30
1	A	140	ASP	CB-CG-OD2	6.04	123.74	118.30
1	A	307	ASP	CB-CG-OD2	5.92	123.63	118.30
1	C	299	ASP	CB-CG-OD2	5.85	123.57	118.30
1	D	151	PRO	N-CA-CB	5.85	110.32	103.30
1	C	301	ASN	N-CA-C	5.75	126.51	111.00
1	C	99	HIS	N-CA-C	5.74	126.49	111.00
1	B	299	ASP	CB-CG-OD2	5.61	123.35	118.30
1	C	167	ASP	CB-CG-OD2	5.57	123.31	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	291	ASP	CB-CG-OD2	5.42	123.18	118.30
1	C	235	ASP	CB-CG-OD2	5.26	123.04	118.30
1	A	282	LEU	CA-CB-CG	-5.15	103.45	115.30
1	B	340	ASP	CB-CG-OD2	5.09	122.88	118.30
1	A	92	LYS	N-CA-CB	5.07	119.73	110.60
1	A	341	ASP	CB-CG-OD2	5.07	122.86	118.30
1	A	106	ASP	CB-CG-OD2	5.06	122.86	118.30
1	D	119	ASP	CB-CG-OD2	5.05	122.85	118.30
1	A	235	ASP	CB-CG-OD2	5.02	122.81	118.30
1	D	185	ASP	CB-CG-OD2	5.00	122.80	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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	2650	0	2594	63	0
1	B	2423	0	2347	68	0
1	C	2619	0	2573	82	0
1	D	476	0	403	9	0
2	A	5	0	0	0	0
2	C	5	0	0	0	0
3	A	8	0	14	2	0
3	C	8	0	14	1	0
4	A	15	0	0	0	0
4	B	6	0	0	0	0
4	C	25	0	0	1	0
4	D	1	0	0	0	0
All	All	8241	0	7945	220	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 14.

All (220) 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:346:GLY:HA2	1:C:371:ASN:HD22	0.99	1.09
1:A:137:THR:HG22	1:A:390:ARG:HH22	1.16	1.03
1:C:346:GLY:HA2	1:C:371:ASN:ND2	1.75	0.99
1:A:261:ASN:O	1:A:261:ASN:ND2	2.04	0.91
1:C:186:GLU:HG2	1:C:189:ILE:HD12	1.57	0.86
1:C:94:PHE:HB3	1:C:99:HIS:CE1	2.11	0.85
1:B:115:SER:OG	1:B:132:ARG:NH2	2.12	0.83
1:A:268:VAL:HB	1:A:271:LYS:HG3	1.60	0.82
1:A:193:PHE:HE2	1:A:262:LYS:HG2	1.44	0.81
1:B:127:LEU:HD21	1:B:156:MET:HE3	1.64	0.79
1:C:203:GLY:H	1:C:302:THR:CG2	1.93	0.79
1:A:137:THR:HG22	1:A:390:ARG:NH2	1.94	0.79
1:B:384:LYS:O	1:B:388:ARG:HB2	1.82	0.79
1:C:133:THR:O	1:C:390:ARG:NH1	2.21	0.73
1:B:114:PHE:HZ	1:B:129:LEU:HD22	1.55	0.72
1:A:150:PHE:CZ	1:B:175:PRO:HG2	2.25	0.72
1:C:186:GLU:HG2	1:C:189:ILE:CD1	2.19	0.72
1:A:174:TYR:CD1	1:A:404:HIS:HB3	2.25	0.71
1:C:116:LEU:HD22	1:C:156:MET:HE1	1.72	0.71
1:C:386:GLU:HG2	3:C:9004:MPD:O4	1.91	0.71
1:A:86:THR:HA	1:A:89:ILE:HD12	1.73	0.70
1:A:340:ASP:OD1	1:A:340:ASP:N	2.21	0.70
1:B:127:LEU:HD21	1:B:156:MET:CE	2.24	0.68
1:B:292:ILE:HD11	1:B:376:CYS:HB2	1.74	0.68
1:A:215:GLU:HA	1:A:215:GLU:OE1	1.92	0.68
1:A:363:GLU:O	1:A:367:THR:HG23	1.93	0.67
1:B:391:ALA:O	1:B:395:GLU:HG3	1.93	0.67
1:C:94:PHE:HD2	1:C:99:HIS:HE1	1.42	0.67
1:C:193:PHE:HE1	1:C:262:LYS:HG2	1.60	0.66
1:C:78:LYS:O	1:C:78:LYS:HD3	1.95	0.66
1:A:341:ASP:OD2	1:A:379:ALA:HB1	1.96	0.66
1:C:94:PHE:HB3	1:C:99:HIS:HE1	1.61	0.66
1:A:347:PRO:HD2	1:A:368:LYS:HD3	1.77	0.65
1:C:202:LEU:HD23	1:C:302:THR:HG23	1.77	0.65
1:C:203:GLY:H	1:C:302:THR:HG21	1.61	0.65
1:B:114:PHE:CZ	1:B:129:LEU:HD22	2.31	0.65
1:A:115:SER:OG	1:A:132:ARG:NH2	2.31	0.64
1:C:384:LYS:NZ	1:C:387:GLU:HG2	2.13	0.64
1:A:245:VAL:HG12	1:A:246:THR:HG23	1.79	0.63
1:C:384:LYS:HZ1	1:C:387:GLU:HG2	1.63	0.63
1:C:116:LEU:HD22	1:C:156:MET:CE	2.28	0.63
1:C:94:PHE:CD2	1:C:99:HIS:HE1	2.15	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:207:GLU:OE1	1:A:285:LYS:HE3	1.99	0.62
1:C:115:SER:OG	1:C:132:ARG:NH2	2.31	0.62
1:A:331:LEU:HD13	1:A:354:VAL:HG11	1.82	0.62
1:B:363:GLU:O	1:B:367:THR:HG23	2.00	0.62
1:C:346:GLY:CA	1:C:371:ASN:HD22	1.93	0.62
1:B:203:GLY:H	1:B:302:THR:HG21	1.64	0.62
1:A:193:PHE:CE2	1:A:262:LYS:HG2	2.32	0.61
1:C:97:LYS:C	1:D:97:LYS:O	2.39	0.61
1:B:224:LEU:HD21	1:B:268:VAL:HG11	1.83	0.61
1:C:79:VAL:HG22	1:C:80:LYS:N	2.16	0.60
1:A:346:GLY:HA2	1:A:371:ASN:HD22	1.66	0.60
1:B:332:TYR:HE2	1:B:357:LYS:HB2	1.66	0.60
1:C:103:TYR:CE1	1:C:170:TYR:HB2	2.37	0.59
1:A:103:TYR:OH	1:A:402:HIS:HD2	1.86	0.59
1:D:404:HIS:HA	1:D:407:SER:HB2	1.85	0.59
1:B:182:VAL:O	1:B:186:GLU:HB2	2.03	0.58
1:C:94:PHE:HD2	1:C:99:HIS:CE1	2.21	0.58
1:B:153:VAL:HG13	1:B:154:VAL:N	2.18	0.57
1:C:188:VAL:O	1:C:188:VAL:CG1	2.52	0.57
1:B:346:GLY:HA2	1:B:371:ASN:HD22	1.70	0.57
1:D:401:LEU:O	1:D:405:SER:HB2	2.06	0.56
1:C:223:PHE:O	1:C:226:PHE:HB3	2.05	0.55
1:A:244:ASP:HB2	1:A:250:THR:HG23	1.88	0.55
1:B:116:LEU:HD13	1:B:156:MET:CE	2.38	0.54
1:B:106:ASP:C	1:B:108:ALA:H	2.11	0.54
1:D:152:ASN:HD22	1:D:152:ASN:H	1.55	0.54
1:B:281:GLN:HG3	1:B:284:ARG:HD2	1.89	0.54
1:C:203:GLY:H	1:C:302:THR:HG23	1.71	0.54
1:B:272:LEU:HB3	1:B:273:PRO:HD2	1.89	0.54
1:B:320:VAL:HG22	1:B:334:VAL:HG22	1.88	0.54
1:B:101:ASN:O	1:B:172:VAL:HG23	2.07	0.54
1:B:357:LYS:O	1:B:357:LYS:HG3	2.06	0.54
1:C:351:ASP:C	1:C:353:ALA:N	2.61	0.53
1:D:174:TYR:HB3	1:D:177:ALA:HB2	1.90	0.53
1:B:288:ILE:O	1:B:291:ASP:HB2	2.08	0.53
1:A:268:VAL:CB	1:A:271:LYS:HG3	2.36	0.52
1:C:92:LYS:HB3	1:C:93:HIS:CD2	2.44	0.52
1:C:345:PHE:O	1:C:346:GLY:O	2.27	0.52
1:B:154:VAL:O	1:B:157:ALA:N	2.41	0.52
1:B:301:ASN:OD1	1:B:302:THR:N	2.43	0.52
1:C:351:ASP:O	1:C:352:PRO:C	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:132:ARG:NH1	1:B:185:ASP:OD1	2.33	0.52
1:A:234:GLN:O	1:A:245:VAL:O	2.28	0.52
1:C:244:ASP:HB3	1:C:250:THR:HG23	1.90	0.52
1:A:388:ARG:HG2	1:A:388:ARG:HH11	1.75	0.51
1:A:145:SER:O	1:A:147:LEU:N	2.44	0.51
1:C:349:LEU:HD23	1:C:364:PHE:CZ	2.46	0.51
1:A:377:TYR:CD2	3:A:9003:MPD:HM2	2.46	0.51
1:B:116:LEU:HD13	1:B:156:MET:HE2	1.93	0.51
1:B:140:ASP:HB2	1:B:160:VAL:HG23	1.93	0.51
1:C:234:GLN:O	1:C:245:VAL:O	2.29	0.51
1:A:302:THR:HG22	1:A:303:PRO:HD2	1.92	0.51
1:B:208:GLU:O	1:B:212:SER:HB3	2.10	0.50
1:C:245:VAL:O	1:C:245:VAL:CG1	2.60	0.50
1:C:79:VAL:CG2	1:C:80:LYS:N	2.74	0.50
1:C:283:GLN:HA	1:C:283:GLN:NE2	2.26	0.50
1:C:86:THR:CG2	1:C:86:THR:O	2.59	0.50
1:A:132:ARG:NH1	1:A:185:ASP:OD1	2.40	0.50
1:A:351:ASP:HB2	1:A:352:PRO:HD3	1.93	0.49
1:C:116:LEU:HD13	1:C:156:MET:HE1	1.94	0.49
1:C:203:GLY:N	1:C:302:THR:HG21	2.26	0.49
1:C:305:VAL:HG23	1:C:306:PRO:HD2	1.93	0.49
1:C:345:PHE:HB3	1:C:375:ALA:HB2	1.93	0.49
1:B:345:PHE:HB3	1:B:375:ALA:HB2	1.93	0.49
1:B:346:GLY:HA3	1:B:368:LYS:HD2	1.95	0.49
1:A:208:GLU:HG3	1:A:279:ALA:HB1	1.94	0.49
1:B:372:ALA:O	1:B:376:CYS:SG	2.68	0.49
1:C:172:VAL:HA	1:C:405:SER:OG	2.11	0.49
1:A:125:GLU:HB2	1:A:144:ILE:CG2	2.43	0.49
1:A:253:GLU:OE2	1:A:271:LYS:HE2	2.13	0.48
1:A:129:LEU:HD11	1:A:142:ILE:HD11	1.95	0.48
1:B:106:ASP:HB2	1:B:112:LEU:HD13	1.96	0.48
1:C:244:ASP:CB	1:C:250:THR:HG23	2.43	0.48
1:C:401:LEU:O	1:C:405:SER:HB2	2.13	0.48
1:D:170:TYR:HB3	1:D:402:HIS:HE1	1.77	0.48
1:C:205:THR:O	1:C:308:MET:HG2	2.14	0.48
1:C:86:THR:O	1:C:86:THR:HG22	2.13	0.48
1:A:200:GLN:HG3	1:A:210:LEU:HD21	1.94	0.48
1:A:331:LEU:HB3	1:A:354:VAL:HG13	1.96	0.48
1:A:286:ARG:NH1	1:A:286:ARG:HG3	2.29	0.48
1:A:333:LYS:HG2	1:A:354:VAL:HG22	1.95	0.48
1:C:200:GLN:OE1	1:C:304:PHE:HB2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:350:PRO:HG2	1:A:353:ALA:HA	1.96	0.47
1:C:106:ASP:HB2	1:C:112:LEU:HD11	1.95	0.47
1:A:377:TYR:CE2	3:A:9003:MPD:H11	2.49	0.47
1:B:113:VAL:HG21	1:B:397:LEU:HD23	1.96	0.47
1:C:191:ASN:HA	1:C:262:LYS:HG3	1.95	0.47
1:B:397:LEU:O	1:B:401:LEU:HG	2.15	0.47
1:D:170:TYR:CB	1:D:402:HIS:CE1	2.97	0.47
1:C:174:TYR:HA	1:C:175:PRO:HD2	1.66	0.47
1:C:127:LEU:HD21	1:C:156:MET:HE3	1.96	0.47
1:B:152:ASN:O	1:B:156:MET:HG3	2.15	0.46
1:B:197:VAL:HB	1:B:268:VAL:HA	1.96	0.46
1:B:281:GLN:NE2	1:B:281:GLN:HA	2.29	0.46
1:B:202:LEU:HD12	1:B:302:THR:HG23	1.98	0.46
1:B:132:ARG:HG2	1:B:137:THR:HG22	1.97	0.46
1:B:142:ILE:HD11	1:B:159:LEU:HB3	1.96	0.46
1:B:319:VAL:O	1:B:334:VAL:HA	2.16	0.46
1:C:301:ASN:CG	1:C:301:ASN:O	2.53	0.46
1:A:193:PHE:CZ	1:A:370:ILE:HG23	2.51	0.46
1:C:305:VAL:HG22	1:C:307:ASP:H	1.80	0.46
1:B:138:TYR:HB3	1:B:160:VAL:HG22	1.98	0.46
1:C:363:GLU:O	1:C:367:THR:HG23	2.16	0.46
1:B:106:ASP:C	1:B:108:ALA:N	2.69	0.45
1:B:203:GLY:N	1:B:302:THR:HG21	2.31	0.45
1:C:347:PRO:HA	1:C:348:PRO:HD2	1.81	0.45
1:B:115:SER:HB2	1:B:130:LEU:HB3	1.98	0.45
1:A:144:ILE:HD12	1:A:144:ILE:HA	1.81	0.45
1:C:349:LEU:HD23	1:C:364:PHE:HZ	1.80	0.45
1:B:101:ASN:ND2	1:B:115:SER:OG	2.50	0.45
1:B:295:VAL:HG22	1:B:369:LEU:HD21	1.98	0.45
1:C:136:ARG:HG3	1:C:137:THR:O	2.16	0.45
1:C:206:SER:O	1:C:210:LEU:HB2	2.17	0.45
1:A:173:LEU:O	1:A:175:PRO:HD3	2.18	0.44
1:A:345:PHE:CE2	1:A:372:ALA:HB2	2.53	0.44
1:C:305:VAL:O	1:C:308:MET:HB2	2.18	0.44
1:A:142:ILE:HD13	1:A:159:LEU:HD13	2.00	0.44
1:A:255:VAL:O	1:A:266:PHE:HB2	2.17	0.44
1:B:106:ASP:HB3	1:B:109:LEU:H	1.82	0.44
1:A:305:VAL:O	1:A:308:MET:HG3	2.18	0.44
1:C:150:PHE:HA	1:C:151:PRO:HD3	1.87	0.44
1:C:171:PRO:HB2	1:C:173:LEU:HD21	2.00	0.44
1:A:239:PHE:HB2	1:A:263:GLU:OE1	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:262:LYS:HG2	1:B:262:LYS:H	1.46	0.44
1:C:133:THR:O	1:C:135:CYS:N	2.51	0.44
1:C:102:TYR:HB3	1:C:169:PHE:HB3	2.00	0.43
1:A:113:VAL:O	1:A:132:ARG:HB2	2.19	0.43
1:A:384:LYS:HG3	1:A:385:LEU:H	1.83	0.43
1:B:388:ARG:HH12	1:B:392:ALA:HB2	1.82	0.43
1:C:304:PHE:CD1	1:C:304:PHE:C	2.92	0.43
1:A:127:LEU:HD21	1:A:156:MET:SD	2.59	0.43
1:B:342:VAL:HA	1:B:343:PRO:HD3	1.74	0.43
1:A:245:VAL:O	1:A:245:VAL:HG13	2.19	0.43
1:C:188:VAL:O	1:C:188:VAL:HG13	2.17	0.43
1:B:259:PHE:CE2	1:B:367:THR:HG22	2.54	0.43
1:A:304:PHE:C	1:A:304:PHE:CD1	2.92	0.43
1:B:115:SER:HG	1:B:132:ARG:HH22	1.64	0.43
1:C:194:LYS:HA	1:C:265:MET:O	2.19	0.43
1:C:365:LEU:HD12	1:C:365:LEU:HA	1.86	0.42
1:D:404:HIS:C	1:D:406:GLN:H	2.21	0.42
1:A:90:TYR:HD1	1:A:182:VAL:HB	1.84	0.42
1:B:106:ASP:HB2	1:B:112:LEU:CD1	2.50	0.42
1:A:217:SER:HB3	1:A:220:PHE:HB2	2.00	0.42
1:B:361:PHE:CD1	1:B:361:PHE:C	2.92	0.42
1:C:393:LEU:HD23	1:C:393:LEU:HA	1.81	0.42
1:C:157:ALA:O	1:C:160:VAL:HG23	2.19	0.42
1:C:200:GLN:HG2	1:C:298:GLN:HG2	2.01	0.42
1:A:231:VAL:HG21	1:A:236:PHE:CE1	2.54	0.42
1:B:388:ARG:NH1	1:B:392:ALA:HB2	2.35	0.42
1:C:106:ASP:HB3	1:C:109:LEU:HB2	2.02	0.42
1:C:306:PRO:C	1:C:308:MET:N	2.73	0.41
1:A:168:ARG:HD3	1:A:170:TYR:OH	2.20	0.41
1:B:184:PHE:C	1:B:184:PHE:CD1	2.93	0.41
1:A:302:THR:HG22	1:A:303:PRO:CD	2.49	0.41
1:A:302:THR:CG2	1:A:303:PRO:HD2	2.50	0.41
1:C:168:ARG:HB3	1:C:168:ARG:HH11	1.84	0.41
1:B:356:ARG:O	1:B:361:PHE:HB2	2.20	0.41
1:B:407:SER:HA	1:B:411:LEU:O	2.21	0.41
1:C:186:GLU:CG	1:C:189:ILE:HD12	2.38	0.41
1:A:286:ARG:HH11	1:A:286:ARG:HG3	1.84	0.41
1:B:153:VAL:HG13	1:B:154:VAL:H	1.86	0.41
1:C:306:PRO:O	1:C:308:MET:N	2.54	0.41
1:C:380:GLU:HG3	4:C:54:HOH:O	2.19	0.41
1:D:397:LEU:O	1:D:401:LEU:HG	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:275:THR:H	1:C:281:GLN:HE22	1.68	0.41
1:A:267:HIS:ND1	1:A:291:ASP:OD2	2.44	0.41
1:C:306:PRO:C	1:C:308:MET:H	2.23	0.41
1:C:345:PHE:CE2	1:C:372:ALA:HB2	2.56	0.41
1:B:153:VAL:CG1	1:B:154:VAL:N	2.83	0.41
1:B:332:TYR:CD2	1:B:361:PHE:HE2	2.39	0.41
1:A:223:PHE:O	1:A:226:PHE:HB3	2.21	0.40
1:A:345:PHE:HB3	1:A:375:ALA:HB2	2.03	0.40
1:C:403:ILE:HG22	1:C:404:HIS:N	2.36	0.40
1:B:251:GLY:CA	1:B:273:PRO:HD3	2.52	0.40
1:B:292:ILE:HA	1:B:314:LEU:HA	2.03	0.40
1:A:346:GLY:HA2	1:A:371:ASN:ND2	2.35	0.40
1:B:82:GLU:OE1	1:B:371:ASN:HB3	2.20	0.40
1:B:109:LEU:HD13	1:B:133:THR:HG21	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	324/341 (95%)	301 (93%)	20 (6%)	3 (1%)	17 48
1	B	292/341 (86%)	258 (88%)	27 (9%)	7 (2%)	6 22
1	C	318/341 (93%)	296 (93%)	18 (6%)	4 (1%)	12 37
1	D	54/341 (16%)	41 (76%)	12 (22%)	1 (2%)	8 28
All	All	988/1364 (72%)	896 (91%)	77 (8%)	15 (2%)	10 34

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	146	CYS

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Mol	Chain	Res	Type
1	B	82	GLU
1	B	261	ASN
1	B	80	LYS
1	B	353	ALA
1	C	301	ASN
1	C	346	GLY
1	A	410	GLY
1	B	346	GLY
1	C	234	GLN
1	A	260	ARG
1	B	290	ASN
1	C	134	LYS
1	D	152	ASN
1	B	107	THR

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	286/301 (95%)	242 (85%)	44 (15%)	2	8
1	B	255/301 (85%)	193 (76%)	62 (24%)	0	2
1	C	284/301 (94%)	228 (80%)	56 (20%)	1	4
1	D	43/301 (14%)	28 (65%)	15 (35%)	0	0
All	All	868/1204 (72%)	691 (80%)	177 (20%)	1	3

All (177) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	79	VAL
1	A	80	LYS
1	A	81	LEU
1	A	92	LYS
1	A	117	LYS
1	A	119	ASP
1	A	124	GLN

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Mol	Chain	Res	Type
1	A	125	GLU
1	A	131	LEU
1	A	134	LYS
1	A	136	ARG
1	A	137	THR
1	A	142	ILE
1	A	145	SER
1	A	150	PHE
1	A	153	VAL
1	A	162	GLU
1	A	166	VAL
1	A	167	ASP
1	A	168	ARG
1	A	180	LEU
1	A	188	VAL
1	A	191	ASN
1	A	201	LYS
1	A	213	THR
1	A	215	GLU
1	A	224	LEU
1	A	234	GLN
1	A	261	ASN
1	A	262	LYS
1	A	269	SER
1	A	271	LYS
1	A	285	LYS
1	A	299	ASP
1	A	308	MET
1	A	337	THR
1	A	340	ASP
1	A	341	ASP
1	A	351	ASP
1	A	357	LYS
1	A	362	GLN
1	A	384	LYS
1	A	385	LEU
1	A	388	ARG
1	B	81	LEU
1	B	86	THR
1	B	92	LYS
1	B	104	SER
1	B	105	LEU

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Mol	Chain	Res	Type
1	B	136	ARG
1	B	145	SER
1	B	152	ASN
1	B	158	LYS
1	B	159	LEU
1	B	162	GLU
1	B	163	ASP
1	B	166	VAL
1	B	167	ASP
1	B	168	ARG
1	B	185	ASP
1	B	186	GLU
1	B	187	HIS
1	B	201	LYS
1	B	202	LEU
1	B	208	GLU
1	B	212	SER
1	B	213	THR
1	B	215	GLU
1	B	224	LEU
1	B	227	LEU
1	B	229	GLN
1	B	231	VAL
1	B	240	ARG
1	B	254	SER
1	B	259	PHE
1	B	262	LYS
1	B	264	ILE
1	B	265	MET
1	B	271	LYS
1	B	280	GLN
1	B	281	GLN
1	B	286	ARG
1	B	292	ILE
1	B	299	ASP
1	B	302	THR
1	B	305	VAL
1	B	311	SER
1	B	321	GLN
1	B	333	LYS
1	B	340	ASP
1	B	341	ASP

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Mol	Chain	Res	Type
1	B	342	VAL
1	B	355	PHE
1	B	357	LYS
1	B	360	GLU
1	B	361	PHE
1	B	363	GLU
1	B	365	LEU
1	B	376	CYS
1	B	378	LYS
1	B	381	LYS
1	B	385	LEU
1	B	388	ARG
1	B	397	LEU
1	B	400	GLU
1	B	409	MET
1	C	77	THR
1	C	78	LYS
1	C	80	LYS
1	C	89	ILE
1	C	92	LYS
1	C	95	LEU
1	C	97	LYS
1	C	99	HIS
1	C	109	LEU
1	C	120	VAL
1	C	134	LYS
1	C	160	VAL
1	C	168	ARG
1	C	179	ARG
1	C	190	SER
1	C	191	ASN
1	C	200	GLN
1	C	202	LEU
1	C	205	THR
1	C	210	LEU
1	C	213	THR
1	C	224	LEU
1	C	227	LEU
1	C	233	LEU
1	C	237	LYS
1	C	240	ARG
1	C	245	VAL

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Mol	Chain	Res	Type
1	C	246	THR
1	C	258	ASN
1	C	262	LYS
1	C	276	GLU
1	C	299	ASP
1	C	300	GLU
1	C	302	THR
1	C	305	VAL
1	C	308	MET
1	C	321	GLN
1	C	337	THR
1	C	341	ASP
1	C	342	VAL
1	C	356	ARG
1	C	357	LYS
1	C	362	GLN
1	C	363	GLU
1	C	378	LYS
1	C	384	LYS
1	C	385	LEU
1	C	386	GLU
1	C	387	GLU
1	C	390	ARG
1	C	396	THR
1	C	399	GLU
1	C	400	GLU
1	C	403	ILE
1	C	407	SER
1	C	409	MET
1	D	93	HIS
1	D	115	SER
1	D	116	LEU
1	D	119	ASP
1	D	152	ASN
1	D	153	VAL
1	D	176	LYS
1	D	181	ILE
1	D	185	ASP
1	D	397	LEU
1	D	399	GLU
1	D	403	ILE
1	D	404	HIS

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Mol	Chain	Res	Type
1	D	405	SER
1	D	409	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	234	GLN
1	A	258	ASN
1	A	261	ASN
1	A	287	HIS
1	A	402	HIS
1	B	84	ASN
1	B	101	ASN
1	B	192	ASN
1	B	312	ASN
1	C	99	HIS
1	C	192	ASN
1	C	283	GLN
1	D	99	HIS
1	D	101	ASN
1	D	152	ASN

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)

4 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	$\#\|Z\| > 2$
3	MPD	C	9004	-	7,7,7	0.85	0	9,10,10	0.48	0
2	SO4	A	9001	-	4,4,4	0.25	0	6,6,6	0.94	0
2	SO4	C	9002	-	4,4,4	0.21	0	6,6,6	0.61	0
3	MPD	A	9003	-	7,7,7	0.70	0	9,10,10	0.74	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	MPD	C	9004	-	-	0/5/5/5	-
3	MPD	A	9003	-	-	0/5/5/5	-

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.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	9004	MPD	1	0
3	A	9003	MPD	2	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	330/341 (96%)	-0.41	8 (2%) 59 56	16, 23, 26, 29	0
1	B	304/341 (89%)	-0.06	10 (3%) 46 41	20, 23, 25, 26	0
1	C	324/341 (95%)	-0.43	3 (0%) 84 84	18, 23, 26, 31	0
1	D	66/341 (19%)	0.62	11 (16%) 1 1	20, 22, 23, 24	0
All	All	1024/1364 (75%)	-0.24	32 (3%) 49 44	16, 23, 26, 31	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	412	GLY	5.3
1	A	146	CYS	4.5
1	D	131	LEU	4.0
1	A	325	GLY	4.0
1	A	413	GLY	3.7
1	D	129	LEU	3.7
1	A	147	LEU	3.6
1	A	411	LEU	3.3
1	D	119	ASP	3.2
1	B	351	ASP	3.1
1	C	77	THR	3.0
1	B	354	VAL	2.9
1	B	350	PRO	2.8
1	C	121	ILE	2.8
1	D	120	VAL	2.8
1	A	407	SER	2.6
1	D	170	TYR	2.6
1	C	122	GLY	2.5
1	B	358	GLY	2.5
1	B	258	ASN	2.5
1	D	398	TYR	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	380	GLU	2.3
1	D	97	LYS	2.3
1	D	90	TYR	2.2
1	D	399	GLU	2.2
1	B	356	ARG	2.1
1	B	121	ILE	2.1
1	B	122	GLY	2.1
1	D	403	ILE	2.0
1	B	282	LEU	2.0
1	A	324	GLY	2.0
1	D	130	LEU	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	MPD	C	9004	8/8	0.81	0.20	75,77,78,78	0
3	MPD	A	9003	8/8	0.93	0.21	75,78,81,81	0
2	SO4	A	9001	5/5	0.97	0.14	72,72,73,75	0
2	SO4	C	9002	5/5	0.99	0.06	72,73,76,77	0

6.5 Other polymers (i)

There are no such residues in this entry.