



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 07:59 PM UTC

PDB ID : 1SRQ / pdb_00001srq
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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

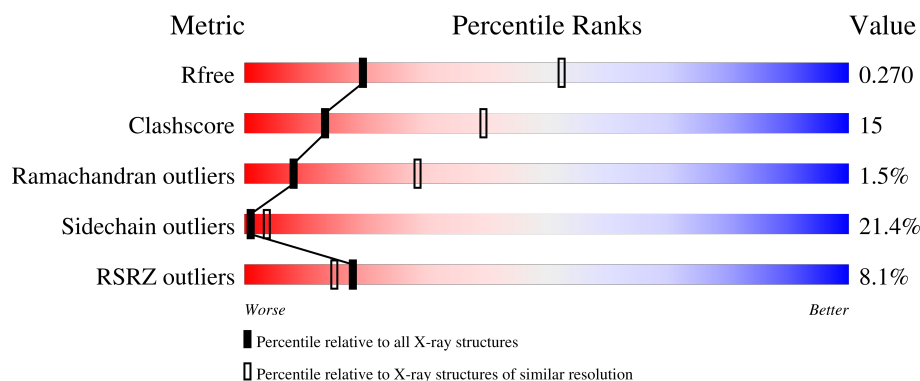
1 Overall quality at a glance

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}	180053	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (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 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 $\leq 5\%$. 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	4% 60% 28% 8% ..
1	B	341	8% 49% 32% 8% 11%
1	C	341	3% 56% 29% 9% 5%
1	D	341	9% 12% 6% 81%

2 Entry composition [i](#)

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 (CCD ID: SO4) (formula: O₄S).



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 (CCD ID: MPD) (formula: C₆H₁₄O₂).



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

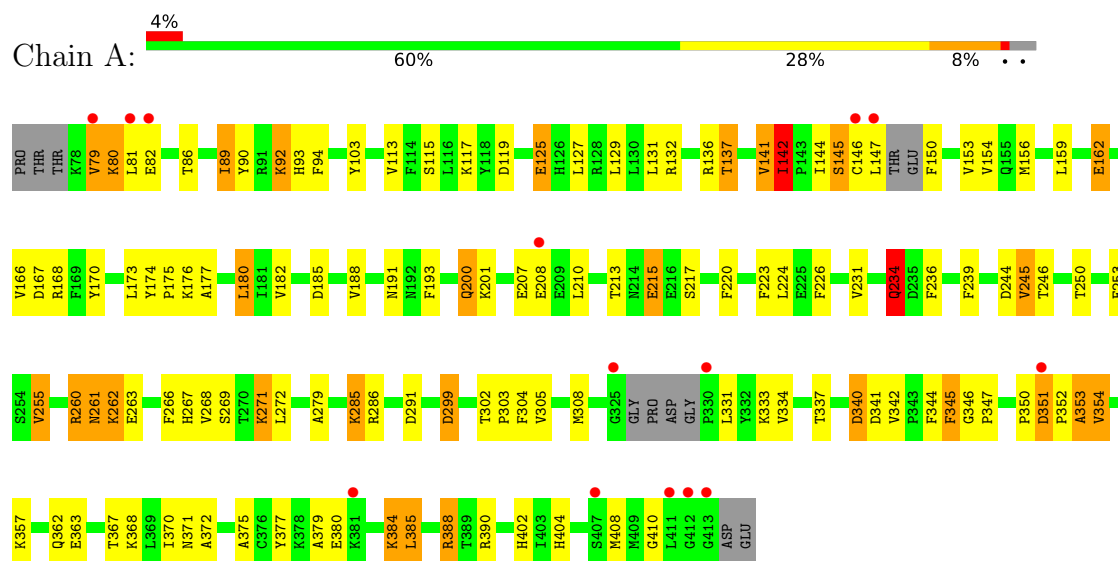
- Molecule 4 is water.

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

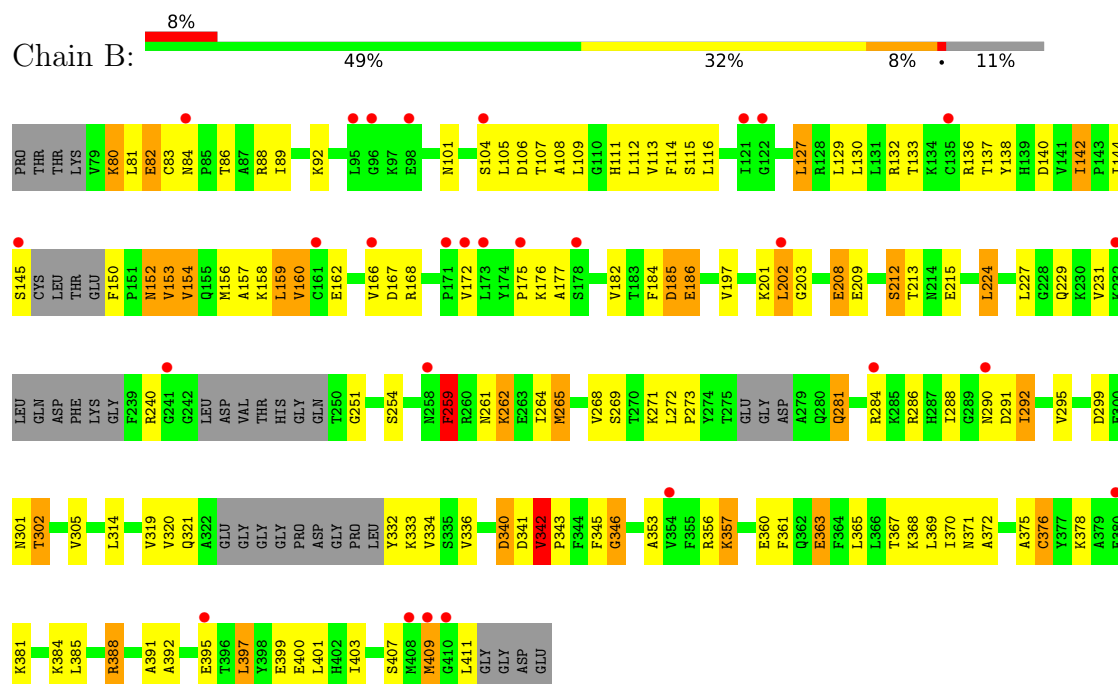
3 Residue-property plots [i](#)

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.

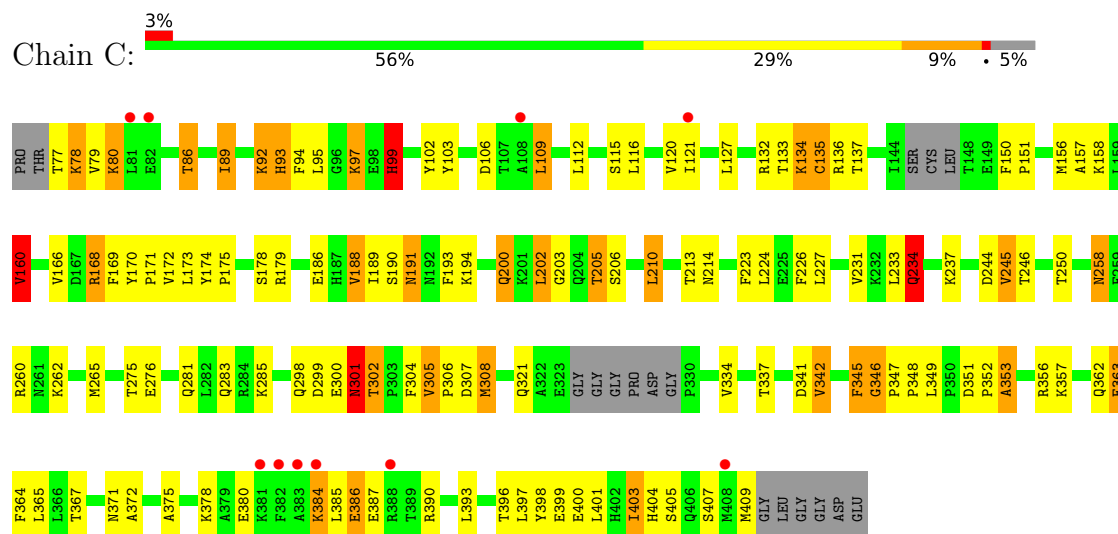
• Molecule 1: GTPase-activating protein 1



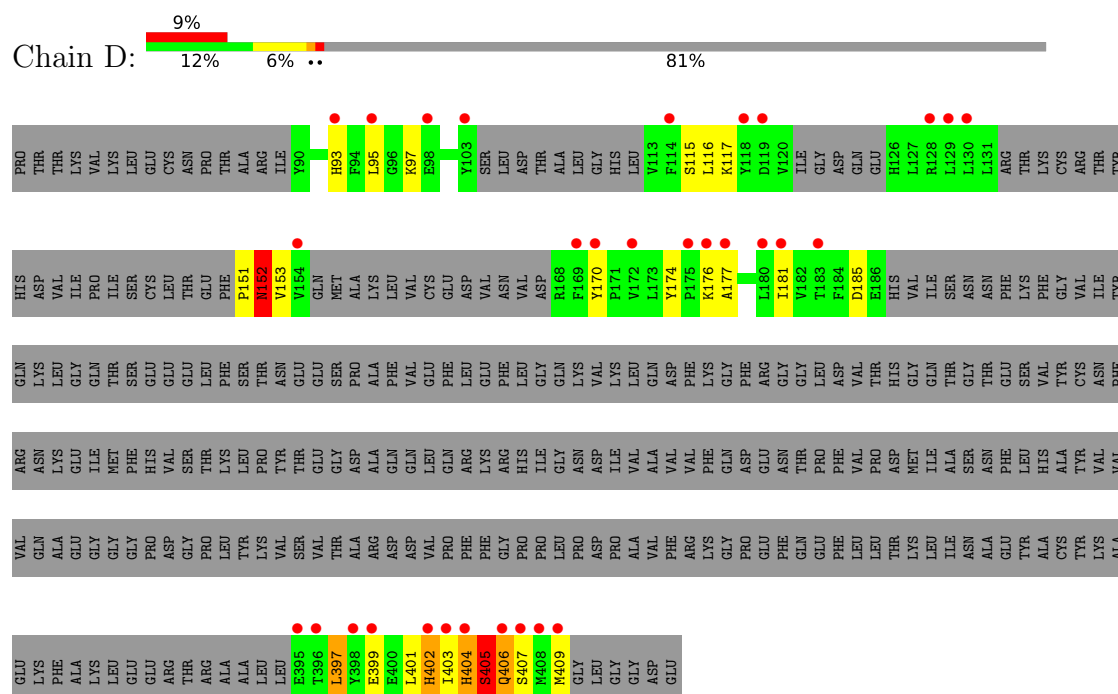
• Molecule 1: GTPase-activating protein 1



- Molecule 1: GTPase-activating protein 1



- Molecule 1: GTPase-activating protein 1



4 Data and refinement statistics

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) 98.5 (14.99-2.90)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.40 (at 2.91Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.232 , 0.276 0.228 , 0.270	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)	0.24 , 51.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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	1.00	1/2714 (0.0%)	1.30	21/3670 (0.6%)
1	B	0.74	3/2481 (0.1%)	1.13	11/3357 (0.3%)
1	C	0.92	1/2683 (0.0%)	1.26	16/3630 (0.4%)
1	D	0.68	0/481	1.13	5/649 (0.8%)
All	All	0.89	5/8359 (0.1%)	1.23	53/11306 (0.5%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	409	MET	SD-CE	8.11	1.99	1.79
1	A	89	ILE	C-N	7.84	1.44	1.33
1	B	88	ARG	C-N	7.45	1.43	1.33
1	B	265	MET	SD-CE	5.94	1.94	1.79
1	C	135	CYS	CA-C	-5.58	1.47	1.53

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	99	HIS	N-CA-C	10.75	126.49	109.50
1	B	342	VAL	N-CA-C	9.45	117.30	107.76
1	C	353	ALA	N-CA-C	9.01	123.57	112.58
1	C	342	VAL	N-CA-C	8.80	117.77	107.73
1	D	402	HIS	N-CA-C	8.49	120.16	111.07
1	C	334	VAL	N-CA-C	7.63	118.80	108.11
1	A	79	VAL	N-CA-C	7.54	120.34	108.87
1	C	234	GLN	CA-C-N	-7.54	111.94	123.17
1	C	234	GLN	C-N-CA	-7.54	111.94	123.17
1	C	301	ASN	N-CA-C	7.38	126.51	110.80
1	A	94	PHE	N-CA-C	6.72	121.72	112.04
1	D	151	PRO	N-CA-CB	6.65	110.32	103.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	89	ILE	N-CA-C	6.60	117.36	110.62
1	A	92	LYS	N-CA-CB	6.47	119.73	110.16
1	C	160	VAL	CB-CA-C	-6.46	103.80	111.94
1	A	92	LYS	N-CA-C	6.43	118.37	111.36
1	B	142	ILE	N-CA-C	6.37	114.91	107.77
1	A	234	GLN	CA-C-N	-6.18	114.74	123.03
1	A	234	GLN	C-N-CA	-6.18	114.74	123.03
1	B	259	PHE	N-CA-C	6.17	120.54	111.34
1	A	89	ILE	O-C-N	-6.11	115.92	121.91
1	A	353	ALA	N-CA-C	6.08	123.74	110.80
1	A	142	ILE	N-CA-C	5.96	114.38	107.89
1	C	345	PHE	N-CA-C	5.86	116.01	108.34
1	A	162	GLU	N-CA-C	5.82	118.37	111.33
1	B	88	ARG	CA-C-N	5.81	128.42	120.46
1	B	88	ARG	C-N-CA	5.81	128.42	120.46
1	D	95	LEU	N-CA-C	5.77	113.51	108.78
1	A	334	VAL	N-CA-C	5.69	116.67	108.48
1	C	260	ARG	CA-C-N	-5.68	113.65	123.25
1	C	260	ARG	C-N-CA	-5.68	113.65	123.25
1	C	214	ASN	N-CA-C	5.67	119.71	112.12
1	A	345	PHE	N-CA-C	5.59	117.47	109.14
1	C	89	ILE	N-CA-C	5.58	116.22	110.36
1	A	180	LEU	N-CA-C	-5.51	105.17	111.07
1	A	299	ASP	N-CA-C	-5.44	106.77	113.41
1	A	82	GLU	N-CA-C	5.42	122.35	110.80
1	D	406	GLN	N-CA-C	-5.42	107.21	113.88
1	A	141	VAL	CA-C-N	-5.41	117.48	123.43
1	A	141	VAL	C-N-CA	-5.41	117.48	123.43
1	C	258	ASN	CA-C-N	-5.40	115.16	121.64
1	C	258	ASN	C-N-CA	-5.40	115.16	121.64
1	B	340	ASP	CA-C-N	5.38	127.44	120.44
1	B	340	ASP	C-N-CA	5.38	127.44	120.44
1	B	177	ALA	N-CA-C	5.32	116.88	111.14
1	B	160	VAL	CB-CA-C	5.31	115.73	111.06
1	A	93	HIS	N-CA-C	5.31	120.24	113.55
1	C	93	HIS	N-CA-C	5.30	120.02	113.50
1	B	153	VAL	N-CA-C	5.19	115.62	110.23
1	D	405	SER	N-CA-C	-5.18	107.03	113.19
1	A	154	VAL	N-CA-C	-5.16	105.36	110.62
1	A	80	LYS	N-CA-C	5.03	117.33	110.24
1	A	260	ARG	N-CA-C	-5.00	100.14	110.80

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	2650	0	2594	71	0
1	B	2423	0	2347	74	0
1	C	2619	0	2573	87	0
1	D	476	0	403	10	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	239	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 15.

All (239) 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:ND2	1:A:261:ASN:O	2.04	0.91
1:C:186:GLU:HG2	1:C:189:ILE:HD12	1.57	0.86
1:B:116:LEU:HD13	1:B:156:MET:HE1	1.55	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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:116:LEU:HD22	1:C:156:MET:HE2	1.71	0.73
1:B:127:LEU:HD11	1:B:156:MET:HE3	1.70	0.72
1:A:150:PHE:CZ	1:B:175:PRO:HG2	2.25	0.72
1:B:114:PHE:HZ	1:B:129:LEU:HD22	1.55	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: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:OE1	1:A:215:GLU:HA	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:C:127:LEU:HD21	1:C:156:MET:HE3	1.76	0.66
1:A:341:ASP:OD2	1:A:379:ALA:HB1	1.96	0.66
1:C:97:LYS:C	1:D:97:LYS:O	2.39	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:94:PHE:CD2	1:C:99:HIS:HE1	2.15	0.63
1:C:116:LEU:HD22	1:C:156:MET:CE	2.28	0.63
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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:384:LYS:HZ1	1:C:387:GLU:HG2	1.66	0.60
1:B:106:ASP:C	1:B:108:ALA:H	2.11	0.59
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:351:ASP:C	1:C:353:ALA:N	2.61	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:C:351:ASP:O	1:C:352:PRO:C	2.45	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:C:116:LEU:HD13	1:C:156:MET:HE1	1.89	0.55
1:D:152:ASN:H	1:D:152:ASN:HD22	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:B:127:LEU:HD21	1:B:156:MET:HE3	1.90	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:304:PHE:CD2	1:A:308:MET:HE2	2.44	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: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:HH11	1:A:388:ARG:HG2	1.75	0.51
1:B:127:LEU:HD21	1:B:156:MET:HE2	1.91	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:377:TYR:CD2	3:A:9003:MPD:HM2	2.46	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:C:301:ASN:O	1:C:301:ASN:CG	2.53	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:B:106:ASP:C	1:B:108:ALA:N	2.69	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: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:404:HIS:C	1:D:406:GLN:H	2.21	0.48
1:D:170:TYR:HB3	1:D:402:HIS:HE1	1.77	0.48
1:A:210:LEU:HD11	1:A:308:MET:HE3	1.95	0.48
1:C:86:THR:O	1:C:86:THR:HG22	2.13	0.48
1:C:205:THR:O	1:C:308:MET:HG2	2.14	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:C:304:PHE:CD1	1:C:304:PHE:C	2.92	0.48
1:A:286:ARG:HG3	1:A:286:ARG:NH1	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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:304:PHE:CD1	1:A:304:PHE:C	2.92	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:202:LEU:HD12	1:B:302:THR:HG23	1.98	0.46
1:B:281:GLN:NE2	1:B:281:GLN:HA	2.29	0.46
1:B:361:PHE:CD1	1:B:361:PHE:C	2.92	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:184:PHE:CD1	1:B:184:PHE:C	2.93	0.46
1:B:319:VAL:O	1:B:334:VAL:HA	2.16	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:C:306:PRO:C	1:C:308:MET:N	2.73	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:C:306:PRO:C	1:C:308:MET:H	2.23	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:261:ASN:ND2	1:A:261:ASN:C	2.74	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:D:404:HIS:C	1:D:406:GLN:N	2.75	0.44
1:B:111:HIS:C	1:B:112:LEU:HD12	2.43	0.44
1:A:305:VAL:O	1:A:308:MET:HG3	2.18	0.44
1:B:116:LEU:HD13	1:B:156:MET:CE	2.38	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:B:262:LYS:H	1:B:262:LYS:HG2	1.46	0.44
1:C:133:THR:O	1:C:135:CYS:N	2.51	0.44
1:C:78:LYS:HD3	1:C:78:LYS:C	2.42	0.43
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:C:364:PHE:CD1	1:C:364:PHE:C	2.96	0.43
1:B:388:ARG:HH12	1:B:392:ALA:HB2	1.82	0.43
1:C:397:LEU:O	1:C:398:TYR:C	2.61	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:A:344:PHE:CD1	1:A:344:PHE:C	2.96	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: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: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:C:393:LEU:HD23	1:C:393:LEU:HA	1.81	0.42
1:A:150:PHE:CD1	1:A:150:PHE:C	2.96	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:408:MET:HE1	1:B:150:PHE:HE1	1.83	0.42
1:A:176:LYS:O	1:A:177:ALA:C	2.61	0.42
1:A:231:VAL:HG21	1:A:236:PHE:CE1	2.54	0.42
1:A:379:ALA:O	1:A:380:GLU:C	2.63	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:A:168:ARG:HD3	1:A:170:TYR:OH	2.20	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:B:115:SER:HG	1:B:132:ARG:HH22	1.65	0.41
1:C:168:ARG:HH11	1:C:168:ARG:HB3	1.84	0.41
1:B:268:VAL:O	1:B:269:SER:C	2.63	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:186:GLU:CG	1:C:189:ILE:HD12	2.38	0.41
1:A:286:ARG:HG3	1:A:286:ARG:HH11	1.84	0.41
1:B:153:VAL:HG13	1:B:154:VAL:H	1.86	0.41
1:C:186:GLU:C	1:C:188:VAL:N	2.76	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
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: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:C:345:PHE:CE2	1:C:372:ALA:HB2	2.56	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:83:CYS:O	1:B:84:ASN:C	2.64	0.40
1:C:186:GLU:C	1:C:188:VAL:H	2.29	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%)	14	41
1	B	292/341 (86%)	258 (88%)	27 (9%)	7 (2%)	4	18
1	C	318/341 (93%)	296 (93%)	18 (6%)	4 (1%)	9	32

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	54/341 (16%)	41 (76%)	12 (22%)	1 (2%)	6	23
All	All	988/1364 (72%)	896 (91%)	77 (8%)	15 (2%)	8	28

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	146	CYS
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 ⓘ

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%)	241 (84%)	45 (16%)	2	9
1	B	255/301 (85%)	189 (74%)	66 (26%)	0	2
1	C	284/301 (94%)	224 (79%)	60 (21%)	1	4
1	D	43/301 (14%)	28 (65%)	15 (35%)	0	0
All	All	868/1204 (72%)	682 (79%)	186 (21%)	1	4

All (186) 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	125	GLU
1	A	131	LEU
1	A	136	ARG
1	A	137	THR
1	A	141	VAL
1	A	142	ILE
1	A	145	SER
1	A	153	VAL
1	A	162	GLU
1	A	166	VAL
1	A	167	ASP
1	A	180	LEU
1	A	188	VAL
1	A	191	ASN
1	A	200	GLN
1	A	201	LYS
1	A	213	THR
1	A	215	GLU
1	A	224	LEU
1	A	234	GLN
1	A	245	VAL
1	A	255	VAL
1	A	261	ASN
1	A	262	LYS
1	A	269	SER
1	A	271	LYS
1	A	272	LEU
1	A	285	LYS
1	A	299	ASP
1	A	337	THR
1	A	340	ASP
1	A	342	VAL
1	A	351	ASP
1	A	354	VAL
1	A	357	LYS
1	A	362	GLN
1	A	384	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	385	LEU
1	A	388	ARG
1	B	80	LYS
1	B	81	LEU
1	B	86	THR
1	B	92	LYS
1	B	104	SER
1	B	105	LEU
1	B	127	LEU
1	B	136	ARG
1	B	144	ILE
1	B	145	SER
1	B	152	ASN
1	B	154	VAL
1	B	158	LYS
1	B	159	LEU
1	B	162	GLU
1	B	166	VAL
1	B	167	ASP
1	B	168	ARG
1	B	176	LYS
1	B	185	ASP
1	B	186	GLU
1	B	201	LYS
1	B	202	LEU
1	B	208	GLU
1	B	209	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	281	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	286	ARG
1	B	292	ILE
1	B	299	ASP
1	B	302	THR
1	B	305	VAL
1	B	321	GLN
1	B	333	LYS
1	B	336	VAL
1	B	340	ASP
1	B	341	ASP
1	B	342	VAL
1	B	357	LYS
1	B	360	GLU
1	B	363	GLU
1	B	365	LEU
1	B	370	ILE
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	399	GLU
1	B	400	GLU
1	B	403	ILE
1	B	409	MET
1	C	77	THR
1	C	78	LYS
1	C	80	LYS
1	C	86	THR
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	121	ILE
1	C	134	LYS
1	C	158	LYS
1	C	160	VAL
1	C	166	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	168	ARG
1	C	178	SER
1	C	179	ARG
1	C	188	VAL
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	231	VAL
1	C	233	LEU
1	C	237	LYS
1	C	245	VAL
1	C	246	THR
1	C	258	ASN
1	C	276	GLU
1	C	285	LYS
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	396	THR
1	C	399	GLU
1	C	400	GLU
1	C	403	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	407	SER
1	C	409	MET
1	D	93	HIS
1	D	115	SER
1	D	116	LEU
1	D	117	LYS
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
1	D	405	SER
1	D	409	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	84	ASN
1	A	155	GLN
1	A	234	GLN
1	A	258	ASN
1	A	261	ASN
1	A	287	HIS
1	A	371	ASN
1	A	402	HIS
1	B	101	ASN
1	B	187	HIS
1	B	192	ASN
1	B	280	GLN
1	B	281	GLN
1	B	287	HIS
1	B	312	ASN
1	B	371	ASN
1	C	99	HIS
1	C	124	GLN
1	C	192	ASN
1	C	298	GLN
1	C	404	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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 oligosaccharides 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	$\# Z > 2$
2	SO4	C	9002	-	4,4,4	0.32	0	6,6,6	0.65	0
2	SO4	A	9001	-	4,4,4	0.35	0	6,6,6	0.81	0
3	MPD	A	9003	-	7,7,7	0.70	0	9,10,10	0.71	0
3	MPD	C	9004	-	7,7,7	0.83	0	9,10,10	0.51	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	A	9003	-	-	0/5/5/5	-
3	MPD	C	9004	-	-	1/5/5/5	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	9004	MPD	C2-C3-C4-C5

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	9003	MPD	2	0
3	C	9004	MPD	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, 95th 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%)	0.02	14 (4%) 40 32	16, 23, 26, 29	0
1	B	304/341 (89%)	0.56	28 (9%) 14 12	20, 23, 25, 26	0
1	C	324/341 (95%)	-0.07	10 (3%) 51 42	18, 23, 26, 31	0
1	D	66/341 (19%)	2.02	31 (46%) 0 0	20, 22, 23, 24	0
All	All	1024/1364 (75%)	0.28	83 (8%) 18 15	16, 23, 26, 31	0

All (83) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	398	TYR	6.6
1	D	409	MET	5.4
1	D	98	GLU	5.4
1	B	96	GLY	5.2
1	B	175	PRO	4.6
1	B	232	LYS	4.6
1	A	146	CYS	4.5
1	B	173	LEU	4.5
1	B	98	GLU	4.4
1	C	381	LYS	4.3
1	C	382	PHE	4.2
1	D	129	LEU	4.1
1	D	128	ARG	4.1
1	C	383	ALA	4.0
1	B	172	VAL	3.8
1	D	154	VAL	3.7
1	C	384	LYS	3.7
1	D	408	MET	3.5
1	C	82	GLU	3.5
1	B	145	SER	3.4
1	D	119	ASP	3.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	258	ASN	3.4
1	D	402	HIS	3.2
1	A	381	LYS	3.2
1	C	81	LEU	3.2
1	D	175	PRO	3.1
1	D	103	TYR	3.0
1	D	118	TYR	3.0
1	D	170	TYR	3.0
1	D	130	LEU	3.0
1	A	208	GLU	3.0
1	D	396	THR	2.9
1	D	404	HIS	2.9
1	B	161	CYS	2.9
1	B	122	GLY	2.9
1	B	95	LEU	2.9
1	B	121	ILE	2.9
1	D	181	ILE	2.8
1	B	178	SER	2.8
1	A	413	GLY	2.8
1	A	411	LEU	2.8
1	B	410	GLY	2.8
1	D	169	PHE	2.7
1	B	171	PRO	2.7
1	C	108	ALA	2.6
1	D	406	GLN	2.6
1	A	325	GLY	2.6
1	D	180	LEU	2.6
1	B	395	GLU	2.6
1	B	84	ASN	2.6
1	B	104	SER	2.5
1	A	412	GLY	2.5
1	A	351	ASP	2.5
1	D	407	SER	2.5
1	A	147	LEU	2.5
1	C	388	ARG	2.5
1	C	121	ILE	2.4
1	B	202	LEU	2.4
1	D	403	ILE	2.4
1	B	354	VAL	2.3
1	D	399	GLU	2.3
1	B	241	GLY	2.3
1	B	408	MET	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	93	HIS	2.3
1	C	408	MET	2.3
1	D	114	PHE	2.2
1	B	409	MET	2.2
1	D	176	LYS	2.2
1	B	380	GLU	2.2
1	A	330	PRO	2.2
1	B	166	VAL	2.2
1	D	395	GLU	2.2
1	B	284	ARG	2.1
1	B	135	CYS	2.1
1	D	172	VAL	2.1
1	D	177	ALA	2.1
1	A	79	VAL	2.1
1	D	183	THR	2.1
1	A	407	SER	2.1
1	A	81	LEU	2.0
1	D	95	LEU	2.0
1	B	290	ASN	2.0
1	A	82	GLU	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 oligosaccharides 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, 95th 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($\text{\AA}^2$)	Q<0.9
3	MPD	C	9004	8/8	0.59	0.19	75,77,78,78	0
3	MPD	A	9003	8/8	0.77	0.16	75,78,81,81	0
2	SO4	A	9001	5/5	0.92	0.11	72,72,73,75	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	SO4	C	9002	5/5	0.96	0.07	72,73,76,77	0

6.5 Other polymers [i](#)

There are no such residues in this entry.