



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 12:19 PM UTC

PDB ID : 3T39 / pdb_00003t39
Title : Crystal structure of the complex of camel peptidoglycan recognition protein(CPGRP-S) with a mycobacterium metabolite shikimate at 2.7 Å resolution
Authors : Sharma, P.; Dube, D.; Sinha, M.; Kaur, P.; Sharma, S.; Singh, T.P.
Deposited on : 2011-07-25
Resolution : 2.70 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

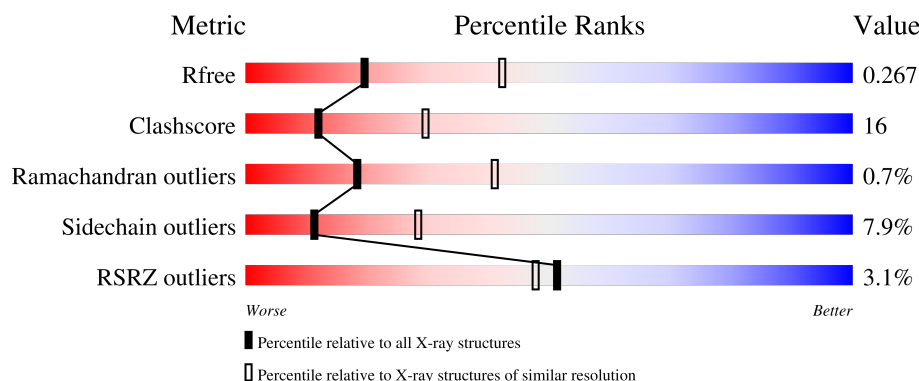
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	171	4% 72% 22% 5%
1	B	171	4% 54% 37% 6%
1	C	171	2% 67% 29% •
1	D	171	2% 60% 33% 6%

2 Entry composition [i](#)

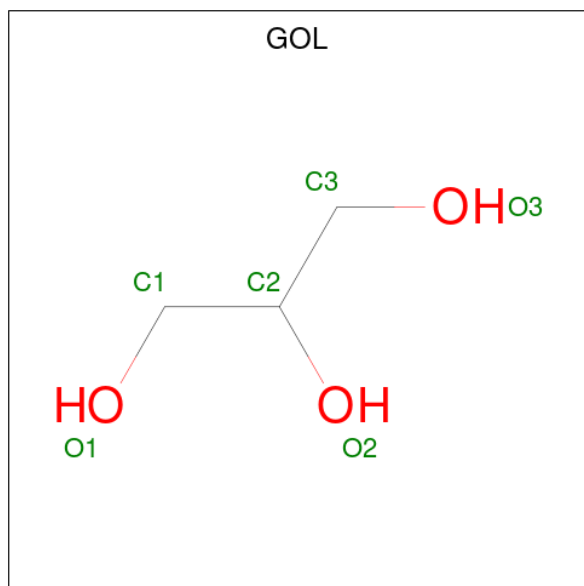
There are 5 unique types of molecules in this entry. The entry contains 5663 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Peptidoglycan recognition protein 1.

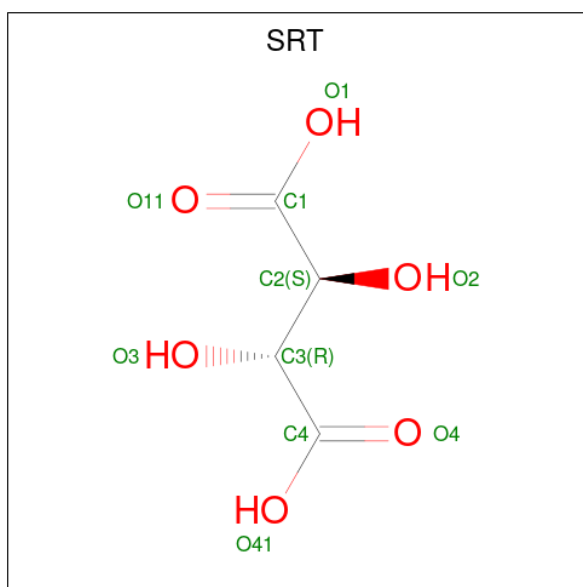
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	171	Total	C	N	O	S	0	0	0
			1336	834	254	240	8			
1	B	171	Total	C	N	O	S	0	0	0
			1336	834	254	240	8			
1	C	171	Total	C	N	O	S	0	0	0
			1336	834	254	240	8			
1	D	171	Total	C	N	O	S	0	0	0
			1336	834	254	240	8			

- Molecule 2 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



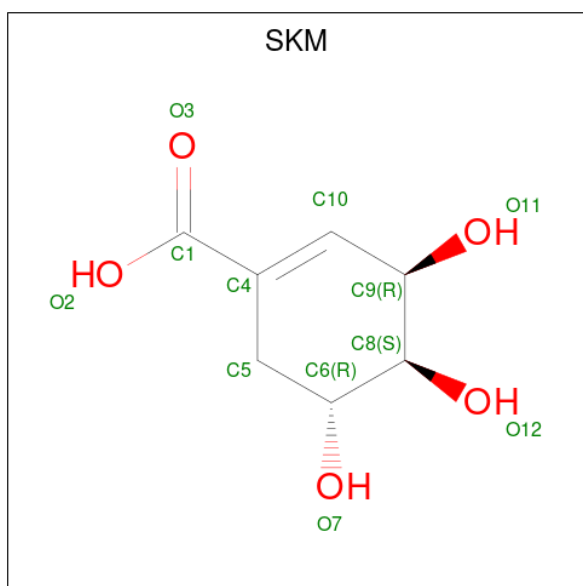
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 3 is S,R MESO-TARTARIC ACID (CCD ID: SRT) (formula: C₄H₆O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	D	1	Total	C	O	0	0
			10	4	6		

- Molecule 4 is (3R,4S,5R)-3,4,5-TRIHIDROXYCYCLOHEX-1-ENE-1-CARBOXYLIC ACID (CCD ID: SKM) (formula: $C_7H_{10}O_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	D	1	Total	C	O	0	0
			12	7	5		

- Molecule 5 is water.

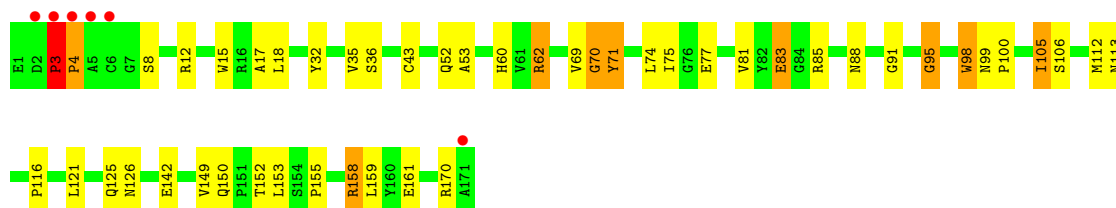
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	85	Total 85	O 85	0	0
5	B	74	Total 74	O 74	0	0
5	C	65	Total 65	O 65	0	0
5	D	67	Total 67	O 67	0	0

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.

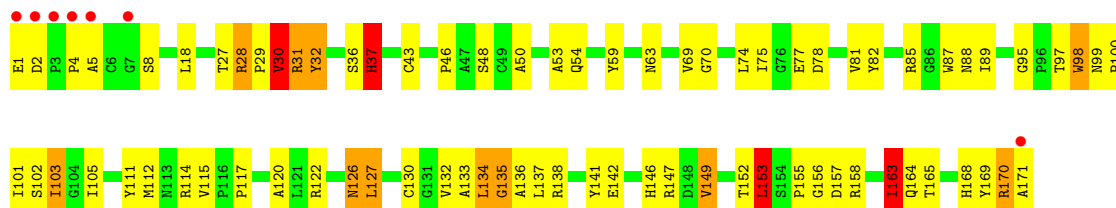
• Molecule 1: Peptidoglycan recognition protein 1

Chain A: 



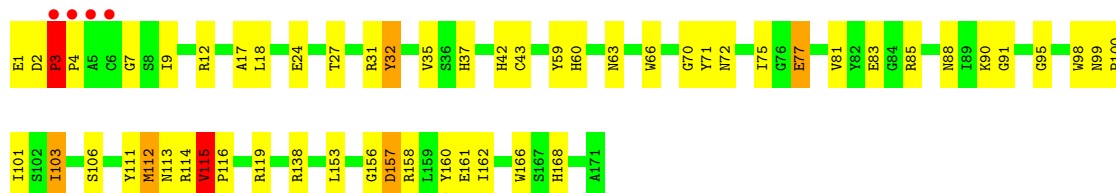
• Molecule 1: Peptidoglycan recognition protein 1

Chain B: 



• Molecule 1: Peptidoglycan recognition protein 1

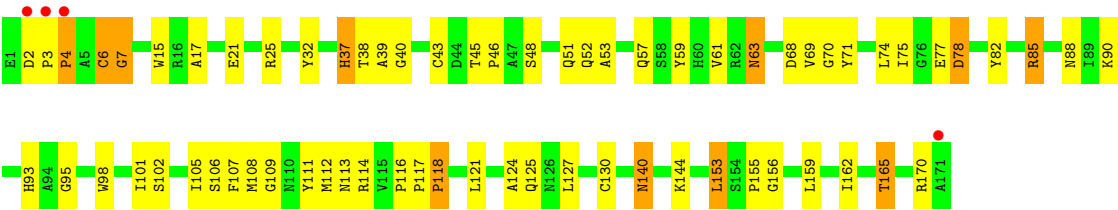
Chain C: 



• Molecule 1: Peptidoglycan recognition protein 1

Chain D: 





4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	89.07Å 101.14Å 163.67Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.02 – 2.70 48.02 – 2.70	Depositor EDS
% Data completeness (in resolution range)	98.8 (48.02-2.70) 98.9 (48.02-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.40 (at 2.69Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.219 , 0.244 0.214 , 0.267	Depositor DCC
R_{free} test set	1045 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	50.7	Xtriage
Anisotropy	0.730	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 41.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	5663	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.42% 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: SRT, SKM, GOL

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	0.61	0/1373	1.25	17/1871 (0.9%)
1	B	0.73	0/1373	1.32	27/1871 (1.4%)
1	C	0.55	0/1373	1.25	21/1871 (1.1%)
1	D	0.59	0/1373	1.31	20/1871 (1.1%)
All	All	0.62	0/5492	1.28	85/7484 (1.1%)

There are no bond length outliers.

All (85) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	3	PRO	N-CA-C	10.31	123.28	110.70
1	D	2	ASP	CA-C-N	9.94	130.61	120.38
1	D	2	ASP	C-N-CA	9.94	130.61	120.38
1	C	18	LEU	N-CA-C	-9.65	96.20	110.48
1	D	78	ASP	N-CA-C	-9.00	102.29	113.18
1	B	31	ARG	N-CA-C	8.86	121.02	111.36
1	D	116	PRO	N-CA-C	-8.66	100.13	110.70
1	D	70	GLY	N-CA-C	8.64	123.10	112.64
1	D	2	ASP	N-CA-C	-8.64	89.55	108.74
1	C	70	GLY	N-CA-C	8.58	123.75	112.77
1	B	5	ALA	N-CA-C	8.51	128.92	110.80
1	B	101	ILE	N-CA-C	8.28	121.03	112.83
1	B	18	LEU	N-CA-C	-8.00	98.64	110.48
1	A	88	ASN	N-CA-C	7.90	123.02	113.23
1	D	6	CYS	N-CA-C	7.79	121.17	108.55
1	C	95	GLY	CA-C-N	7.68	127.73	119.28
1	C	95	GLY	C-N-CA	7.68	127.73	119.28
1	B	70	GLY	N-CA-C	7.60	121.85	112.73
1	C	32	TYR	N-CA-C	7.32	120.86	109.52
1	C	3	PRO	N-CA-C	7.21	119.49	110.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	25	ARG	N-CA-C	7.16	121.52	110.42
1	B	30	VAL	N-CA-C	7.14	119.72	108.87
1	A	4	PRO	CB-CA-C	7.13	120.61	111.56
1	B	50	ALA	N-CA-C	-7.12	103.45	111.14
1	B	153	LEU	N-CA-C	-7.08	104.10	112.89
1	D	88	ASN	N-CA-C	6.99	121.98	113.38
1	C	156	GLY	N-CA-C	-6.94	102.63	111.72
1	B	4	PRO	CB-CA-C	-6.71	100.48	111.56
1	D	3	PRO	CA-C-N	6.67	128.18	119.84
1	D	3	PRO	C-N-CA	6.67	128.18	119.84
1	C	112	MET	N-CA-C	-6.66	103.50	111.69
1	A	71	TYR	N-CA-C	6.52	119.35	110.55
1	C	88	ASN	N-CA-C	6.46	121.45	113.50
1	C	160	TYR	N-CA-C	-6.46	104.24	111.28
1	B	98	TRP	N-CA-C	6.42	121.31	112.90
1	C	37	HIS	N-CA-C	-6.38	100.05	109.81
1	A	116	PRO	N-CA-C	-6.32	102.99	110.70
1	B	53	ALA	N-CA-C	-6.30	104.32	111.07
1	B	37	HIS	N-CA-C	-6.14	99.89	109.72
1	D	93	HIS	N-CA-CB	-6.13	102.88	110.98
1	A	116	PRO	CA-C-N	5.92	123.93	119.66
1	A	116	PRO	C-N-CA	5.92	123.93	119.66
1	C	113	ASN	N-CA-C	5.91	120.20	111.87
1	A	95	GLY	CA-C-N	5.85	125.71	119.28
1	A	95	GLY	C-N-CA	5.85	125.71	119.28
1	B	4	PRO	N-CA-C	5.76	124.33	112.47
1	C	111	TYR	N-CA-C	5.74	120.06	112.25
1	B	115	VAL	N-CA-CB	5.73	115.78	111.83
1	D	85	ARG	N-CA-C	-5.70	106.33	113.28
1	C	115	VAL	N-CA-C	-5.63	96.71	108.88
1	A	98	TRP	N-CA-C	5.58	119.26	112.23
1	A	4	PRO	N-CA-C	5.53	119.89	111.15
1	A	32	TYR	N-CA-C	5.53	118.56	109.72
1	D	7	GLY	N-CA-C	5.53	126.28	113.18
1	A	153	LEU	N-CA-C	-5.47	106.44	113.23
1	B	5	ALA	N-CA-CB	-5.47	101.25	110.49
1	B	88	ASN	N-CA-C	5.44	120.05	113.41
1	C	116	PRO	N-CA-C	-5.43	104.07	110.70
1	D	111	TYR	N-CA-C	5.43	119.64	112.25
1	B	27	THR	N-CA-C	5.42	118.19	108.17
1	D	153	LEU	N-CA-C	-5.41	106.68	113.28
1	B	163	ILE	CB-CA-C	-5.41	103.78	112.16

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	101	ILE	CB-CA-C	-5.37	102.34	111.37
1	A	158	ARG	N-CA-C	5.33	116.90	111.14
1	B	135	GLY	N-CA-C	-5.33	107.18	114.64
1	D	102	SER	N-CA-C	5.28	116.31	108.60
1	A	18	LEU	N-CA-C	-5.28	102.47	110.28
1	C	166	TRP	N-CA-C	5.27	118.12	110.42
1	B	95	GLY	CA-C-N	5.23	124.86	119.05
1	B	95	GLY	C-N-CA	5.23	124.86	119.05
1	A	70	GLY	N-CA-C	5.21	118.98	112.73
1	B	32	TYR	N-CA-C	5.20	118.20	110.14
1	B	78	ASP	N-CA-C	-5.20	106.77	113.01
1	B	120	ALA	N-CA-C	-5.15	105.74	111.36
1	C	157	ASP	N-CA-C	5.15	116.58	111.07
1	C	42	HIS	N-CA-C	5.14	117.94	110.17
1	A	69	VAL	N-CA-C	-5.14	102.22	109.63
1	D	63	ASN	N-CA-C	5.13	118.70	112.23
1	C	168	HIS	N-CA-C	5.13	119.40	113.20
1	B	158	ARG	N-CA-C	5.12	116.86	111.28
1	B	127	LEU	N-CA-C	-5.10	105.42	111.69
1	D	95	GLY	CA-C-N	5.09	124.81	119.82
1	D	95	GLY	C-N-CA	5.09	124.81	119.82
1	C	35	VAL	N-CA-C	5.06	115.98	108.23
1	C	77	GLU	N-CA-C	-5.06	107.08	113.20

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	1336	0	1288	30	0
1	B	1336	0	1288	52	0
1	C	1336	0	1288	33	0
1	D	1336	0	1288	50	0
2	D	6	0	8	1	0
3	D	10	0	3	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	12	0	9	0	0
5	A	85	0	0	0	1
5	B	74	0	0	1	1
5	C	65	0	0	1	0
5	D	67	0	0	0	0
All	All	5663	0	5172	165	1

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 16.

All (165) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:112:MET:HE1	1:D:153:LEU:HB3	1.29	1.11
1:D:74:LEU:HD22	1:D:108:MET:HE3	1.32	1.08
1:B:134:LEU:HD23	1:B:134:LEU:N	1.71	1.05
1:B:112:MET:HE2	1:B:156:GLY:HA2	1.41	1.01
1:B:133:ALA:C	1:B:134:LEU:HD23	2.00	0.87
1:C:112:MET:HE2	1:C:157:ASP:H	1.44	0.82
1:C:75:ILE:HD13	1:C:81:VAL:HG22	1.60	0.82
1:D:75:ILE:HD13	1:D:124:ALA:HB2	1.66	0.78
1:B:29:PRO:HB3	1:B:135:GLY:O	1.82	0.77
1:B:31:ARG:HD3	1:B:32:TYR:CE1	2.20	0.76
1:C:9:ILE:HD12	1:C:81:VAL:CG1	2.17	0.74
1:C:75:ILE:CD1	1:C:81:VAL:HG22	2.17	0.74
1:D:112:MET:CE	1:D:153:LEU:HB3	2.15	0.74
1:A:62:ARG:HH11	1:A:62:ARG:HG3	1.53	0.73
1:A:155:PRO:HB2	1:A:159:LEU:HD23	1.69	0.73
1:D:74:LEU:CD2	1:D:108:MET:HE3	2.17	0.72
1:D:112:MET:HE1	1:D:153:LEU:CB	2.15	0.71
1:A:35:VAL:HG22	1:A:105:ILE:CD1	2.21	0.69
1:B:81:VAL:HG11	1:B:127:LEU:HD13	1.74	0.69
1:A:35:VAL:HG22	1:A:105:ILE:HD11	1.72	0.69
1:D:162:ILE:O	1:D:165:THR:HB	1.95	0.67
1:B:37:HIS:HD2	1:B:111:TYR:H	1.41	0.67
1:D:32:TYR:CD1	1:D:101:ILE:HD13	2.30	0.67
1:B:43:CYS:HB2	1:B:48:SER:OG	1.94	0.66
1:A:3:PRO:N	1:A:4:PRO:HD3	2.10	0.66
1:A:75:ILE:CD1	1:A:81:VAL:HG22	2.26	0.65
1:B:112:MET:CE	1:B:153:LEU:HG	2.25	0.65
1:B:132:VAL:HA	1:B:137:LEU:O	1.96	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:112:MET:HE2	1:D:156:GLY:HA2	1.77	0.65
1:C:31:ARG:HD2	1:C:138:ARG:NH1	2.11	0.64
1:C:12:ARG:HG3	1:C:83:GLU:OE1	1.99	0.62
1:C:43:CYS:O	1:C:77:GLU:HB2	1.99	0.62
1:B:146:HIS:O	1:B:149:VAL:HG12	2.01	0.61
1:C:9:ILE:HD12	1:C:81:VAL:HG11	1.83	0.61
1:B:99:ASN:N	1:B:100:PRO:HD2	2.16	0.60
1:B:122:ARG:O	1:B:126:ASN:HB3	2.01	0.60
1:C:2:ASP:HB3	1:C:3:PRO:CD	2.30	0.60
1:C:112:MET:HE2	1:C:157:ASP:N	2.16	0.60
1:B:37:HIS:CD2	1:B:111:TYR:H	2.20	0.60
1:A:75:ILE:HD12	1:A:81:VAL:HG22	1.82	0.59
1:A:99:ASN:N	1:A:100:PRO:HD2	2.17	0.59
1:D:71:TYR:OH	2:D:503:GOL:H31	2.02	0.59
1:C:31:ARG:HD2	1:C:138:ARG:HH12	1.68	0.59
1:D:38:THR:HG1	1:D:109:GLY:H	1.47	0.59
1:C:59:TYR:HA	1:C:63:ASN:OD1	2.03	0.58
1:B:43:CYS:O	1:B:77:GLU:HB2	2.04	0.58
1:D:53:ALA:HA	1:D:108:MET:HE1	1.86	0.58
1:D:98:TRP:CE3	1:D:101:ILE:HD11	2.39	0.58
1:C:85:ARG:HD2	1:C:91:GLY:HA2	1.86	0.57
1:D:155:PRO:HB2	1:D:159:LEU:HD23	1.85	0.57
1:A:3:PRO:CD	1:A:4:PRO:HD3	2.35	0.57
1:A:62:ARG:HH11	1:A:62:ARG:CG	2.17	0.57
1:B:89:ILE:HD12	1:B:89:ILE:N	2.19	0.56
1:D:75:ILE:HD12	1:D:107:PHE:CE1	2.40	0.56
1:D:140:ASN:H	1:D:140:ASN:HD22	1.53	0.56
1:A:142:GLU:HG2	1:A:170:ARG:HG3	1.89	0.55
1:A:3:PRO:HD2	1:A:4:PRO:HD3	1.89	0.54
1:A:43:CYS:O	1:A:77:GLU:HB2	2.07	0.54
1:B:98:TRP:CE2	1:B:149:VAL:HG22	2.43	0.54
1:D:38:THR:OG1	1:D:108:MET:HA	2.07	0.53
1:D:101:ILE:C	1:D:101:ILE:HD12	2.33	0.53
1:B:75:ILE:N	1:B:75:ILE:HD12	2.24	0.53
1:D:121:LEU:O	1:D:125:GLN:HG3	2.08	0.53
1:D:112:MET:CE	1:D:156:GLY:HA2	2.38	0.53
1:C:32:TYR:CD1	1:C:101:ILE:HD13	2.44	0.52
1:B:99:ASN:N	1:B:100:PRO:CD	2.72	0.52
1:B:112:MET:HE2	1:B:156:GLY:CA	2.27	0.52
1:D:74:LEU:HD22	1:D:108:MET:CE	2.22	0.52
1:B:134:LEU:N	1:B:134:LEU:CD2	2.43	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:87:TRP:CE3	1:B:103:ILE:HD13	2.45	0.51
1:B:141:TYR:O	1:B:168:HIS:HB3	2.11	0.51
1:D:68:ASP:OD1	1:D:69:VAL:N	2.43	0.51
1:A:3:PRO:N	1:A:4:PRO:CD	2.73	0.51
1:B:87:TRP:CZ3	1:B:103:ILE:HD13	2.46	0.51
1:C:12:ARG:HB3	1:C:17:ALA:HB3	1.93	0.51
1:B:77:GLU:HG2	1:B:117:PRO:HD2	1.92	0.51
1:C:60:HIS:O	1:C:66:TRP:HB2	2.11	0.51
1:C:9:ILE:HD13	1:C:81:VAL:HB	1.92	0.50
1:C:2:ASP:C	1:C:4:PRO:HD2	2.36	0.50
1:D:78:ASP:OD2	1:D:82:TYR:OH	2.26	0.50
1:B:112:MET:HE1	1:B:153:LEU:HG	1.93	0.50
1:B:133:ALA:C	1:B:134:LEU:CD2	2.81	0.50
1:C:98:TRP:CE3	1:C:101:ILE:HD11	2.47	0.49
1:D:15:TRP:CH2	1:D:17:ALA:HB2	2.48	0.48
1:D:77:GLU:OE1	1:D:117:PRO:HD3	2.13	0.48
1:C:99:ASN:N	1:C:100:PRO:CD	2.76	0.48
1:B:32:TYR:HB2	1:B:102:SER:CB	2.44	0.48
1:B:163:ILE:HG22	1:B:164:GLN:N	2.23	0.48
1:D:127:LEU:O	1:D:130:CYS:HB3	2.14	0.48
1:D:59:TYR:HD1	1:D:63:ASN:HB2	1.79	0.48
1:A:121:LEU:O	1:A:125:GLN:HG3	2.13	0.47
1:D:57:GLN:O	1:D:61:VAL:HG23	2.14	0.47
1:D:71:TYR:CD2	1:D:106:SER:HB2	2.49	0.47
1:B:98:TRP:C	1:B:100:PRO:HD2	2.39	0.47
1:D:105:ILE:O	1:D:105:ILE:HG13	2.13	0.47
1:B:153:LEU:HD12	1:B:153:LEU:HA	1.82	0.47
1:A:98:TRP:CD1	1:A:149:VAL:HB	2.50	0.46
1:D:52:GLN:O	1:D:53:ALA:C	2.57	0.46
1:A:85:ARG:HD2	1:A:91:GLY:HA2	1.98	0.46
1:D:57:GLN:HG3	1:D:69:VAL:HB	1.97	0.46
1:A:60:HIS:ND1	1:A:70:GLY:N	2.55	0.46
1:A:12:ARG:HG3	1:A:83:GLU:HG2	1.98	0.46
1:B:28:ARG:HA	1:B:29:PRO:HA	1.63	0.46
1:B:169:TYR:CE2	1:B:171:ALA:HB2	2.51	0.46
1:D:38:THR:OG1	1:D:109:GLY:N	2.37	0.46
1:D:140:ASN:HD22	1:D:140:ASN:N	2.15	0.45
1:D:85:ARG:NH1	1:D:90:LYS:O	2.46	0.45
1:D:15:TRP:CZ2	1:D:17:ALA:HB2	2.52	0.45
1:B:147:ARG:C	1:B:149:VAL:H	2.24	0.45
1:B:142:GLU:HB3	1:B:170:ARG:HB2	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:39:ALA:HB2	3:D:172:SRT:O4	2.17	0.45
1:D:45:THR:OG1	1:D:48:SER:HB2	2.17	0.44
1:A:36:SER:HA	1:A:155:PRO:HB3	1.99	0.44
1:B:32:TYR:HB2	1:B:102:SER:HB3	1.99	0.44
1:B:59:TYR:O	1:B:63:ASN:HB2	2.17	0.44
1:D:75:ILE:CD1	1:D:124:ALA:HB2	2.44	0.44
1:C:101:ILE:C	1:C:101:ILE:HD12	2.43	0.44
1:C:9:ILE:CD1	1:C:81:VAL:CG1	2.94	0.44
1:C:9:ILE:CD1	1:C:81:VAL:HB	2.47	0.44
1:B:28:ARG:NH2	5:B:196:HOH:O	2.26	0.44
1:B:74:LEU:HB2	1:B:82:TYR:HB2	2.00	0.44
1:D:112:MET:CE	1:D:153:LEU:CB	2.89	0.44
1:C:71:TYR:CD2	1:C:106:SER:HB2	2.54	0.43
1:A:52:GLN:O	1:A:53:ALA:C	2.61	0.43
1:A:105:ILE:HD13	1:A:105:ILE:O	2.19	0.43
1:D:117:PRO:O	1:D:118:PRO:C	2.62	0.43
1:A:155:PRO:HB2	1:A:159:LEU:CD2	2.45	0.43
1:C:9:ILE:HD13	5:C:216:HOH:O	2.18	0.43
1:A:95:GLY:HA3	1:A:150:GLN:NE2	2.33	0.43
1:A:15:TRP:CZ3	1:A:17:ALA:HB2	2.53	0.43
1:D:59:TYR:O	1:D:63:ASN:HB2	2.19	0.43
1:B:30:VAL:HG11	1:B:103:ILE:HD12	2.01	0.43
1:D:43:CYS:SG	1:D:43:CYS:O	2.77	0.42
1:D:144:LYS:HD3	1:D:170:ARG:O	2.19	0.42
1:B:77:GLU:OE2	1:B:114:ARG:NH2	2.53	0.42
1:B:98:TRP:CD1	1:B:149:VAL:HG22	2.54	0.42
1:D:32:TYR:HD1	1:D:101:ILE:HD13	1.78	0.42
1:B:134:LEU:HA	1:B:134:LEU:HD22	1.44	0.42
1:B:69:VAL:O	1:B:85:ARG:NE	2.43	0.42
1:B:163:ILE:O	1:B:163:ILE:HG23	2.18	0.42
1:C:24:GLU:HB3	1:C:90:LYS:HE2	2.02	0.42
1:C:72:ASN:CG	1:C:103:ILE:CD1	2.92	0.42
1:D:38:THR:C	1:D:40:GLY:H	2.28	0.42
1:B:36:SER:HA	1:B:155:PRO:HB3	2.01	0.42
1:D:37:HIS:C	1:D:37:HIS:CD2	2.98	0.42
1:B:98:TRP:CE2	1:B:149:VAL:CG2	3.02	0.42
1:B:28:ARG:HD3	1:B:136:ALA:HA	2.01	0.42
1:C:158:ARG:O	1:C:161:GLU:HB3	2.20	0.42
1:B:163:ILE:HA	1:B:163:ILE:HD12	1.51	0.41
1:D:38:THR:HG1	1:D:109:GLY:N	2.16	0.41
1:D:6:CYS:HB2	1:D:130:CYS:HB2	2.01	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:9:ILE:HD12	1:C:81:VAL:HG12	1.99	0.41
1:B:147:ARG:NH2	1:B:157:ASP:OD1	2.48	0.41
1:C:103:ILE:HD13	1:C:103:ILE:HA	1.81	0.41
1:B:31:ARG:HA	1:B:138:ARG:HD3	2.01	0.41
1:A:71:TYR:CE2	1:A:106:SER:HB2	2.56	0.41
1:B:137:LEU:HA	1:B:137:LEU:HD23	1.67	0.40
1:C:115:VAL:HG12	1:C:162:ILE:HD11	2.03	0.40
1:C:153:LEU:HD23	1:C:153:LEU:HA	1.88	0.40
1:A:74:LEU:O	1:A:75:ILE:HD13	2.20	0.40
1:A:99:ASN:N	1:A:100:PRO:CD	2.84	0.40
1:A:62:ARG:CG	1:A:62:ARG:NH1	2.80	0.40
1:A:112:MET:O	1:A:158:ARG:HG2	2.22	0.40
1:C:99:ASN:N	1:C:100:PRO:HD3	2.37	0.40
1:D:75:ILE:HD12	1:D:107:PHE:CD1	2.56	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:202:HOH:O	5:B:232:HOH:O[7_454]	1.46	0.74

5.3 Torsion angles

5.3.1 Protein backbone

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	169/171 (99%)	155 (92%)	13 (8%)	1 (1%)	21	44
1	B	169/171 (99%)	149 (88%)	20 (12%)	0	100	100
1	C	169/171 (99%)	159 (94%)	8 (5%)	2 (1%)	10	27
1	D	169/171 (99%)	155 (92%)	12 (7%)	2 (1%)	10	27
All	All	676/684 (99%)	618 (91%)	53 (8%)	5 (1%)	18	41

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	7	GLY
1	D	4	PRO
1	D	7	GLY
1	A	3	PRO
1	C	3	PRO

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	139/139 (100%)	131 (94%)	8 (6%)	18	42
1	B	139/139 (100%)	119 (86%)	20 (14%)	3	8
1	C	139/139 (100%)	133 (96%)	6 (4%)	26	54
1	D	139/139 (100%)	129 (93%)	10 (7%)	13	32
All	All	556/556 (100%)	512 (92%)	44 (8%)	11	28

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	SER
1	A	62	ARG
1	A	83	GLU
1	A	105	ILE
1	A	113	ASN
1	A	126	ASN
1	A	152	THR
1	A	161	GLU
1	B	1	GLU
1	B	2	ASP
1	B	8	SER
1	B	28	ARG
1	B	30	VAL
1	B	37	HIS
1	B	46	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	54	GLN
1	B	97	THR
1	B	103	ILE
1	B	105	ILE
1	B	126	ASN
1	B	130	CYS
1	B	134	LEU
1	B	149	VAL
1	B	152	THR
1	B	153	LEU
1	B	163	ILE
1	B	165	THR
1	B	170	ARG
1	C	1	GLU
1	C	27	THR
1	C	103	ILE
1	C	114	ARG
1	C	115	VAL
1	C	119	ARG
1	D	4	PRO
1	D	21	GLU
1	D	37	HIS
1	D	46	PRO
1	D	51	GLN
1	D	113	ASN
1	D	114	ARG
1	D	118	PRO
1	D	140	ASN
1	D	165	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	150	GLN
1	B	37	HIS
1	B	113	ASN
1	B	140	ASN
1	B	168	HIS
1	C	51	GLN
1	C	52	GLN
1	D	52	GLN
1	D	63	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	93	HIS
1	D	140	ASN
1	D	150	GLN

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](#)

3 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	GOL	D	503	-	5,5,5	0.36	0	5,5,5	0.33	0
4	SKM	D	6873	-	12,12,12	2.74	6 (50%)	16,17,17	2.73	5 (31%)
3	SRT	D	172	-	9,9,9	2.87	4 (44%)	12,12,12	2.11	5 (41%)

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
2	GOL	D	503	-	-	0/4/4/4	-
4	SKM	D	6873	-	-	4/4/20/20	0/1/1/1
3	SRT	D	172	-	-	1/12/12/12	-

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	172	SRT	O2-C2	6.64	1.55	1.42
4	D	6873	SKM	C9-C10	6.16	1.58	1.50
4	D	6873	SKM	C6-C8	4.60	1.59	1.52
3	D	172	SRT	O3-C3	-3.42	1.35	1.42
4	D	6873	SKM	O11-C9	3.23	1.49	1.43
3	D	172	SRT	C2-C1	-2.76	1.48	1.52
3	D	172	SRT	C3-C4	-2.63	1.48	1.52
4	D	6873	SKM	O7-C6	2.47	1.48	1.43
4	D	6873	SKM	C8-C9	2.32	1.57	1.52
4	D	6873	SKM	O3-C1	-2.30	1.17	1.22

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	6873	SKM	O2-C1-C4	7.73	131.76	115.43
4	D	6873	SKM	O3-C1-C4	-5.63	111.77	121.64
3	D	172	SRT	O1-C1-C2	3.83	123.96	113.31
3	D	172	SRT	C3-C2-C1	-3.71	101.59	109.82
4	D	6873	SKM	O2-C1-O3	-3.15	116.40	123.90
4	D	6873	SKM	O12-C8-C6	2.54	115.23	110.05
3	D	172	SRT	O3-C3-C2	-2.45	105.18	110.17
4	D	6873	SKM	O11-C9-C8	-2.18	106.27	110.31
3	D	172	SRT	O2-C2-C3	2.08	114.41	110.17
3	D	172	SRT	O1-C1-O11	-2.05	119.44	124.08

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	6873	SKM	O2-C1-C4-C5
4	D	6873	SKM	O3-C1-C4-C5
4	D	6873	SKM	O2-C1-C4-C10
4	D	6873	SKM	O3-C1-C4-C10
3	D	172	SRT	O2-C2-C3-O3

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	503	GOL	1	0
3	D	172	SRT	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	171/171 (100%)	-0.20	6 (3%)	47	43	30, 47, 63, 100	0
1	B	171/171 (100%)	0.18	7 (4%)	41	37	33, 56, 83, 102	0
1	C	171/171 (100%)	-0.15	4 (2%)	61	58	30, 43, 61, 99	0
1	D	171/171 (100%)	-0.03	4 (2%)	61	58	31, 46, 65, 100	0
All	All	684/684 (100%)	-0.05	21 (3%)	51	48	30, 47, 76, 102	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	5	ALA	4.9
1	D	3	PRO	3.9
1	B	2	ASP	3.6
1	A	3	PRO	3.6
1	A	4	PRO	3.6
1	D	171	ALA	3.2
1	B	5	ALA	3.2
1	B	171	ALA	3.1
1	A	2	ASP	2.9
1	C	6	CYS	2.9
1	B	4	PRO	2.8
1	C	3	PRO	2.8
1	D	2	ASP	2.8
1	B	3	PRO	2.7
1	A	5	ALA	2.7
1	D	4	PRO	2.6
1	B	1	GLU	2.3
1	C	4	PRO	2.3
1	A	6	CYS	2.2
1	A	171	ALA	2.1
1	B	7	GLY	2.1

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
4	SKM	D	6873	12/12	0.67	0.15	96,96,97,97	0
3	SRT	D	172	10/10	0.75	0.18	72,75,76,77	0
2	GOL	D	503	6/6	0.81	0.14	57,58,59,59	0

6.5 Other polymers [i](#)

There are no such residues in this entry.