



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:09 PM GMT

PDB ID : 3T39
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
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

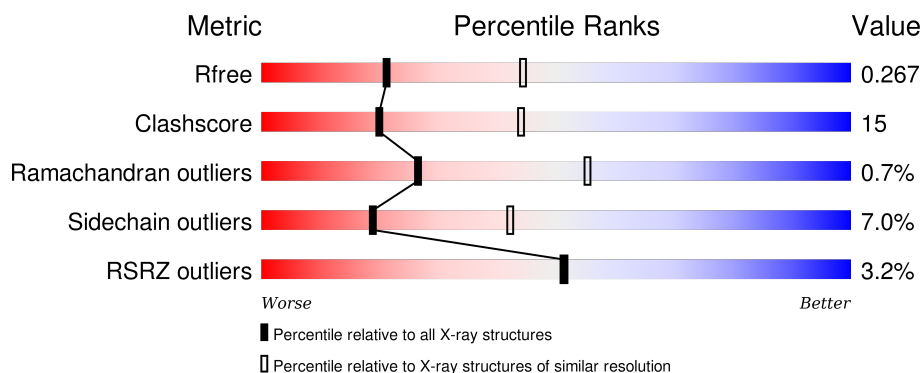
1 Overall quality at a glance

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}	91344	2103 (2.70-2.70)
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	<div> <div>4%</div> <div>76%</div> <div>22%</div> <div>.</div> </div>
1	B	171	<div> <div>5%</div> <div>63%</div> <div>33%</div> <div>5%</div> </div>
1	C	171	<div> <div>3%</div> <div>75%</div> <div>24%</div> <div>..</div> </div>
1	D	171	<div> <div>2%</div> <div>68%</div> <div>30%</div> <div>.</div> </div>

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	GOL	D	503	-	-	-	X
3	SRT	D	172	-	-	-	X

2 Entry composition [i](#)

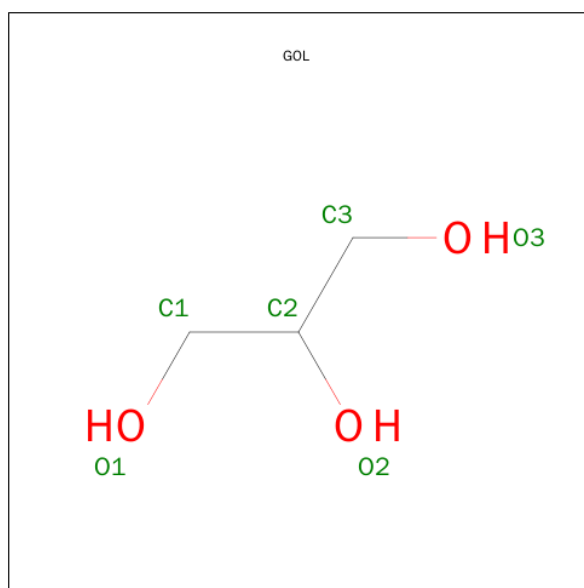
There are 5 unique types of molecules in this entry. The entry contains 5663 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

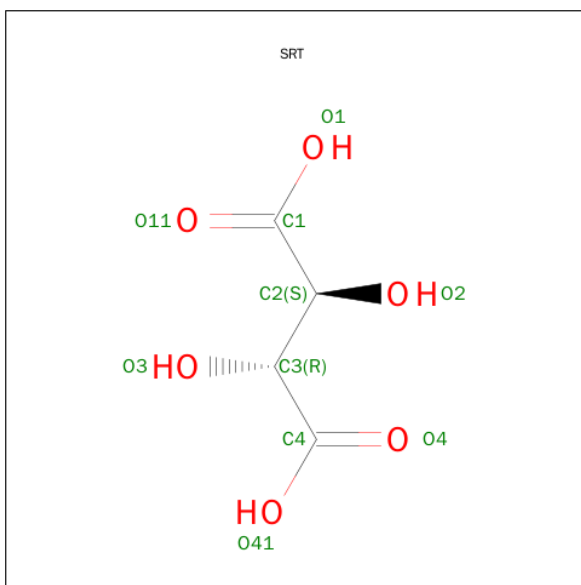
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	171	Total	C	N	O	S	0	0	0
			1336	834	254	240	8			
1	B	171	Total	C	N	O	S	0	0	0
			1336	834	254	240	8			
1	C	171	Total	C	N	O	S	0	0	0
			1336	834	254	240	8			
1	D	171	Total	C	N	O	S	0	0	0
			1336	834	254	240	8			

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



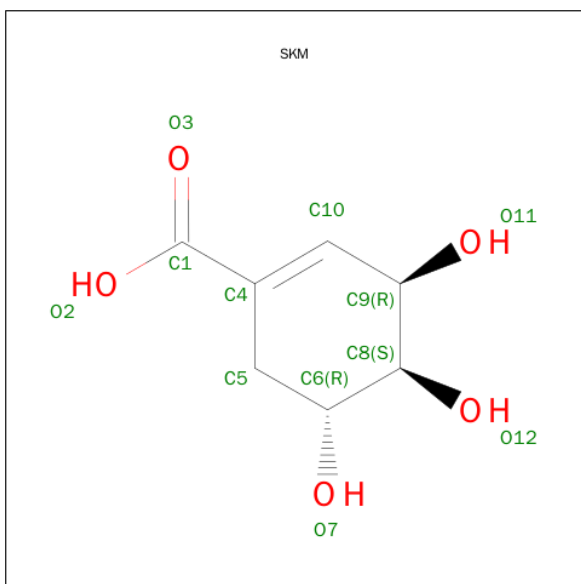
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 3 is S,R MESO-TARTARIC ACID (three-letter code: 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 (three-letter code: 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

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($\text{RSRZ} > 2$). 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.

Chain A:

Label	Color
E1	Green
E2	Green
P3	Green
D3	Green
T152	Green
P4	Green
A5	Green
S8	Green
R12	Green
A15	Green
A16	Green
A17	Green
V35	Green
S36	Green
H37	Green
C43	Green
H60	Green
V61	Green
R62	Orange
G70	Green
Y71	Green
L74	Green
L75	Green
G76	Green
E77	Green
V81	Green
G82	Green
E83	Orange
E84	Green
R85	Green
G91	Green
G95	Green
H98	Green
I99	Green
P100	Green
I105	Orange
S106	Orange
M112	Green
M113	Green
L121	Green
Q125	Green
M126	Green
E142	Green
H140	Green
Q150	Green
P151	Green
T152	Green
P155	Green
R158	Green
L159	Green
Y160	Green
E161	Green
R170	Green
A171	Green

Chain B:

Label	Color
E1	Red
E2	Red
E3	Red
E4	Red
E5	Red
E6	Red
E7	Red
E8	Yellow
E9	Yellow
E10	Yellow
E11	Yellow
E12	Yellow
E13	Yellow
E14	Yellow
E15	Yellow
E16	Yellow
E17	Yellow
E18	Yellow
E19	Yellow
E20	Yellow
E21	Yellow
E22	Yellow
E23	Yellow
E24	Yellow
E25	Yellow
E26	Yellow
E27	Yellow
E28	Yellow
E29	Yellow
E30	Yellow
E31	Yellow
E32	Yellow

Chain C: 

Chain D:

Category	Percentage
E1	2%
D2	0%
P3	0%
P4	0%
A5	0%
A6	0%
C6	0%
G7	0%
W15	0%
R16	0%
A17	0%
E21	0%
Y32	0%
H37	0%
T38	0%
A39	0%
C43	0%
D44	0%
T45	0%
S48	0%
Q51	0%
Q52	0%
A53	0%
Q57	0%
S58	0%
Y59	0%
H60	0%
V61	0%
R62	0%
M63	0%
D68	0%
V69	0%
G70	0%
Y71	0%
L74	0%
I75	0%
G76	0%
E77	0%
D78	0%
Y82	0%
R85	0%
K90	0%
W98	0%
I101	0%
I105	0%

S106	F107	M108	G109
M112	N113	P117	L121
A124	Q125	N126	L127
C130	N140	K144	L153
S154	P155	G156	L159
I162	T169	R170	A171

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 (5.12%)	DCC
Wilson B-factor (Å ²)	50.7	Xtriage
Anisotropy	0.730	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 46.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 20479 reflections	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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SKM, GOL, SRT

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	0.43	0/1373	0.80	0/1871
1	B	0.55	0/1373	0.89	2/1871 (0.1%)
1	C	0.40	0/1373	0.81	2/1871 (0.1%)
1	D	0.43	0/1373	0.84	2/1871 (0.1%)
All	All	0.46	0/5492	0.84	6/7484 (0.1%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	2	ASP	N-CA-C	-7.94	89.55	111.00
1	B	5	ALA	N-CA-C	6.64	128.92	111.00
1	B	5	ALA	N-CA-CB	-6.32	101.25	110.10
1	C	18	LEU	N-CA-C	-5.48	96.20	111.00
1	C	115	VAL	N-CA-C	-5.29	96.71	111.00
1	D	7	GLY	N-CA-C	5.27	126.28	113.10

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	1336	0	1288	29	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1336	0	1288	52	0
1	C	1336	0	1288	31	0
1	D	1336	0	1288	44	0
2	D	6	0	8	1	0
3	D	10	0	3	1	0
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	156	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 15.

All (156) 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:B:134:LEU:N	1:B:134:LEU:HD23	1.71	1.05
1:B:112:MET:HE1	1:B:153:LEU:HG	1.52	0.90
1:D:112:MET:HE1	1:D:153:LEU:HB3	1.56	0.86
1:B:133:ALA:C	1:B:134:LEU:HD23	2.00	0.82
1:C:75:ILE:HD13	1:C:81:VAL:HG22	1.60	0.82
1:D:74:LEU:HD22	1:D:108:MET:HE3	1.64	0.80
1:C:112:MET:HE2	1:C:157:ASP:H	1.49	0.78
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:D:112:MET:CE	1:D:153:LEU:HB3	2.15	0.75
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:A:62:ARG:HG3	1:A:62:ARG:HH11	1.53	0.73
1:A:155:PRO:HB2	1:A:159:LEU:HD23	1.69	0.73
1:B:112:MET:HE2	1:B:156:GLY:HA2	1.71	0.72
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:74:LEU:HD22	1:D:108:MET:CE	2.22	0.68
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:C:9:ILE:HD12	1:C:81:VAL:HG11	1.83	0.61
1:B:146:HIS:O	1:B:149:VAL:HG12	2.01	0.61
1:B:99:ASN:N	1:B:100:PRO:HD2	2.16	0.60
1:C:2:ASP:HB3	1:C:3:PRO:CD	2.30	0.60
1:B:122:ARG:O	1:B:126:ASN:HB3	2.01	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: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:62:ARG:CG	1:A:62:ARG:HH11	2.17	0.57
1:A:3:PRO:CD	1:A:4:PRO:HD3	2.35	0.57
1:D:75:ILE:HD12	1:D:107:PHE:CE1	2.40	0.56
1:B:89:ILE:HD12	1:B:89:ILE:N	2.19	0.56
1:D:140:ASN:HD22	1:D:140:ASN:H	1.53	0.56
1:C:112:MET:HE2	1:C:157:ASP:N	2.20	0.55
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:B:112:MET:CE	1:B:156:GLY:HA2	2.36	0.54
1:D:38:THR:OG1	1:D:108:MET:HA	2.07	0.53
1:D:121:LEU:O	1:D:125:GLN:HG3	2.08	0.53
1:B:75:ILE:N	1:B:75:ILE:HD12	2.24	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:134:LEU:N	1:B:134:LEU:CD2	2.43	0.52
1:B:87:TRP:CE3	1:B:103:ILE:HD13	2.45	0.51
1:D:68:ASP:OD1	1:D:69:VAL:N	2.43	0.51
1:B:141:TYR:O	1:B:168:HIS:HB3	2.11	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:98:TRP:CE3	1:C:101:ILE:HD11	2.47	0.49
1:D:101:ILE:HD12	1:D:101:ILE:C	2.33	0.48
1:D:77:GLU:OE1	1:D:117:PRO:HD3	2.13	0.48
1:D:15:TRP:CH2	1:D:17:ALA:HB2	2.48	0.48
1:C:99:ASN:N	1:C:100:PRO:CD	2.76	0.48
1:D:112:MET:CE	1:D:153:LEU:CB	2.89	0.48
1:B:32:TYR:HB2	1:B:102:SER:CB	2.44	0.48
1:D:127:LEU:O	1:D:130:CYS:HB3	2.14	0.48
1:B:163:ILE:HG22	1:B:164:GLN:N	2.23	0.48
1:D:59:TYR:HD1	1:D:63:ASN:HB2	1.79	0.48
1:D:71:TYR:CD2	1:D:106:SER:HB2	2.49	0.47
1:D:57:GLN:O	1:D:61:VAL:HG23	2.14	0.47
1:A:121:LEU:O	1:A:125:GLN:HG3	2.13	0.47
1:D:105:ILE:HG13	1:D:105:ILE:O	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:57:GLN:HG3	1:D:69:VAL:HB	1.97	0.46
1:A:85:ARG:HD2	1:A:91:GLY:HA2	1.98	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:D:38:THR:OG1	1:D:109:GLY:N	2.37	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:C:2:ASP:C	1:C:4:PRO:HD2	2.36	0.45
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:D:39:ALA:HB2	3:D:172:SRT:O4	2.17	0.45
1:B:142:GLU:HB3	1:B:170:ARG:HB2	1.98	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:75:ILE:CD1	1:D:124:ALA:HB2	2.44	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: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:B:112:MET:HE2	1:B:156:GLY:CA	2.45	0.43
1:C:71:TYR:CD2	1:C:106:SER:HB2	2.54	0.43
1:A:105:ILE:O	1:A:105:ILE:HD13	2.19	0.43
1:C:9:ILE:HD13	5:C:216:HOH:O	2.18	0.43
1:A:155:PRO:HB2	1:A:159:LEU:CD2	2.45	0.43
1:B:98:TRP:C	1:B:100:PRO:HD2	2.39	0.43
1:A:95:GLY:HA3	1:A:150:GLN:NE2	2.33	0.43
1:D:59:TYR:O	1:D:63:ASN:HB2	2.19	0.43
1:A:15:TRP:CZ3	1:A:17:ALA:HB2	2.53	0.43
1:B:30:VAL:HG11	1:B:103:ILE:HD12	2.01	0.43
1:D:144:LYS:HD3	1:D:170:ARG:O	2.19	0.42
1:D:43:CYS:SG	1:D:43:CYS:O	2.77	0.42
1:D:32:TYR:HD1	1:D:101:ILE:HD13	1.78	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:B:134:LEU:HA	1:B:134:LEU:HD22	1.44	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:B:69:VAL:O	1:B:85:ARG:NE	2.43	0.42
1:B:36:SER:HA	1:B:155:PRO:HB3	2.01	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:D:38:THR:HG1	1:D:109:GLY:N	2.16	0.41
1:B:163:ILE:HD12	1:B:163:ILE:HA	1.51	0.41
1:D:52:GLN:O	1:D:53:ALA:C	2.57	0.41
1:D:6:CYS:HB2	1:D:130:CYS:HB2	2.01	0.41
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:D:78:ASP:OD2	1:D:82:TYR:OH	2.26	0.41
1:C:103:ILE:HD13	1:C:103:ILE:HA	1.81	0.41
1:D:112:MET:HE3	1:D:153:LEU:CB	2.51	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:137:LEU:HD23	1:B:137:LEU:HA	1.67	0.40
1:B:147:ARG:C	1:B:149:VAL:H	2.24	0.40
1:C:115:VAL:HG12	1:C:162:ILE:HD11	2.03	0.40
1:C:153:LEU:HA	1:C:153:LEU:HD23	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:D:75:ILE:HD12	1:D:107:PHE:CD1	2.56	0.40
1:A:62:ARG:CG	1:A:62:ARG:NH1	2.80	0.40
1:C:99:ASN:N	1:C:100:PRO:HD3	2.37	0.40
1:A:112:MET:O	1:A:158:ARG:HG2	2.22	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 [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	169/171 (99%)	155 (92%)	13 (8%)	1 (1%)	30	59
1	B	169/171 (99%)	149 (88%)	20 (12%)	0	100	100
1	C	169/171 (99%)	159 (94%)	8 (5%)	2 (1%)	16	39
1	D	169/171 (99%)	155 (92%)	12 (7%)	2 (1%)	16	39
All	All	676/684 (99%)	618 (91%)	53 (8%)	5 (1%)	26	55

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%)	130 (94%)	9 (6%)	21	46
1	B	139/139 (100%)	122 (88%)	17 (12%)	6	14
1	C	139/139 (100%)	133 (96%)	6 (4%)	35	66
1	D	139/139 (100%)	132 (95%)	7 (5%)	30	60
All	All	556/556 (100%)	517 (93%)	39 (7%)	19	42

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	SER
1	A	37	HIS
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	30	VAL
1	B	37	HIS
1	B	97	THR
1	B	103	ILE
1	B	126	ASN

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Mol	Chain	Res	Type
1	B	130	CYS
1	B	134	LEU
1	B	140	ASN
1	B	149	VAL
1	B	152	THR
1	B	158	ARG
1	B	163	ILE
1	B	165	THR
1	B	170	ARG
1	C	27	THR
1	C	37	HIS
1	C	114	ARG
1	C	115	VAL
1	C	116	PRO
1	C	119	ARG
1	D	4	PRO
1	D	21	GLU
1	D	37	HIS
1	D	51	GLN
1	D	113	ASN
1	D	140	ASN
1	D	165	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) 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	C	52	GLN
1	D	63	ASN
1	D	140	ASN

5.3.3 RNA ⓘ

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 carbohydrates 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	$\# Z > 2$
3	SRT	D	172	-	3,9,9	4.12	2 (66%)	6,12,12	2.55	2 (33%)
2	GOL	D	503	-	5,5,5	0.29	0	5,5,5	0.30	0
4	SKM	D	6873	-	10,12,12	2.87	5 (50%)	9,17,17	1.37	1 (11%)

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

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	172	SRT	O3-C3	-3.53	1.35	1.42
4	D	6873	SKM	C8-C9	2.01	1.57	1.52
4	D	6873	SKM	O7-C6	2.29	1.48	1.43
4	D	6873	SKM	O11-C9	2.75	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	6873	SKM	C6-C8	5.11	1.59	1.52
4	D	6873	SKM	C9-C10	6.06	1.58	1.50
3	D	172	SRT	O2-C2	6.15	1.55	1.42

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	172	SRT	C1-C2-C3	-5.73	101.59	113.35
3	D	172	SRT	O2-C2-C3	2.06	114.41	108.61
4	D	6873	SKM	O12-C8-C6	2.90	115.23	110.00

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	172	SRT	1	0
2	D	503	GOL	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%)	-0.04	6 (3%)	48	48	30, 47, 63, 100	0
1	B	171/171 (100%)	0.15	8 (4%)	35	34	33, 56, 83, 102	0
1	C	171/171 (100%)	-0.14	5 (2%)	55	55	30, 43, 61, 99	0
1	D	171/171 (100%)	-0.02	3 (1%)	71	72	31, 46, 65, 100	0
All	All	684/684 (100%)	-0.01	22 (3%)	51	51	30, 47, 76, 102	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	2	ASP	11.7
1	A	2	ASP	10.1
1	A	3	PRO	9.6
1	B	1	GLU	8.8
1	A	4	PRO	7.8
1	C	5	ALA	7.2
1	D	3	PRO	7.1
1	B	4	PRO	6.8
1	D	2	ASP	6.4
1	A	1	GLU	5.3
1	D	1	GLU	5.0
1	B	5	ALA	4.6
1	C	2	ASP	4.6
1	B	3	PRO	4.3
1	C	3	PRO	4.1
1	C	1	GLU	3.8
1	A	5	ALA	3.0
1	A	171	ALA	2.8
1	C	4	PRO	2.6
1	B	170	ARG	2.2
1	B	28	ARG	2.2
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 carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	LLDF	B-factors(\AA^2)	Q<0.9
3	SRT	D	172	10/10	0.84	0.33	8.10	72,75,76,77	0
2	GOL	D	503	6/6	0.85	0.22	4.05	57,58,59,59	0
4	SKM	D	6873	12/12	0.75	0.25	0.18	96,96,97,97	0

6.5 Other polymers [i](#)

There are no such residues in this entry.