



Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 09:03 pm BST

PDB ID : 3CKD
Title : Crystal structure of the C-terminal domain of the Shigella type III effector IpaH
Authors : Lam, R.; Singer, A.U.; Cuff, M.E.; Skarina, T.; Kagan, O.; DiLeo, R.; Edwards, A.M.; Joachimiak, A.; Savchenko, A.; Midwest Center for Structural Genomics (MCSG)
Deposited on : 2008-03-14
Resolution : 2.65 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 : 2.11
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) : 2.11

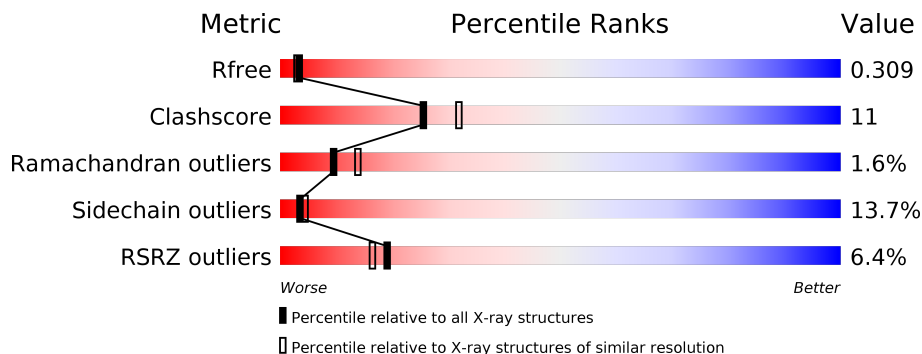
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.65 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	1332 (2.68-2.64)
Clashscore	141614	1374 (2.68-2.64)
Ramachandran outliers	138981	1349 (2.68-2.64)
Sidechain outliers	138945	1349 (2.68-2.64)
RSRZ outliers	127900	1318 (2.68-2.64)

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 $\leq 5\%$. 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	312	7% 55% 23% 6% 16%
1	B	312	8% 61% 12% 5% 22%
1	C	312	% 61% 22% • • 13%

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 6327 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 Invasion plasmid antigen, secreted by the Mxi-Spa secretion machinery.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	262	2114	1319	373	416	1	5	0	0	0
1	B	244	1970	1233	343	389		5	0	0	0
1	C	272	2184	1359	385	434	1	5	0	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	264	GLY	-	EXPRESSION TAG	UNP Q8VSA1
B	264	GLY	-	EXPRESSION TAG	UNP Q8VSA1
C	264	GLY	-	EXPRESSION TAG	UNP Q8VSA1

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



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

- Molecule 4 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C₄H₁₀O₃).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	1	Total C O 7 4 3	0	0

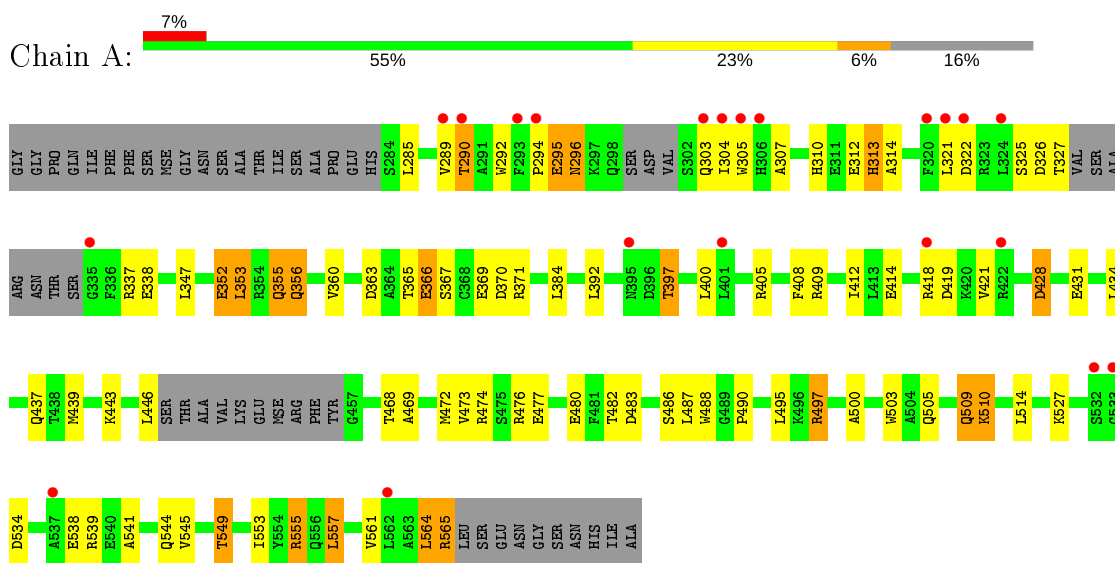
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total O 1 1	0	0
5	B	4	Total O 4 4	0	0
5	C	19	Total O 19 19	0	0

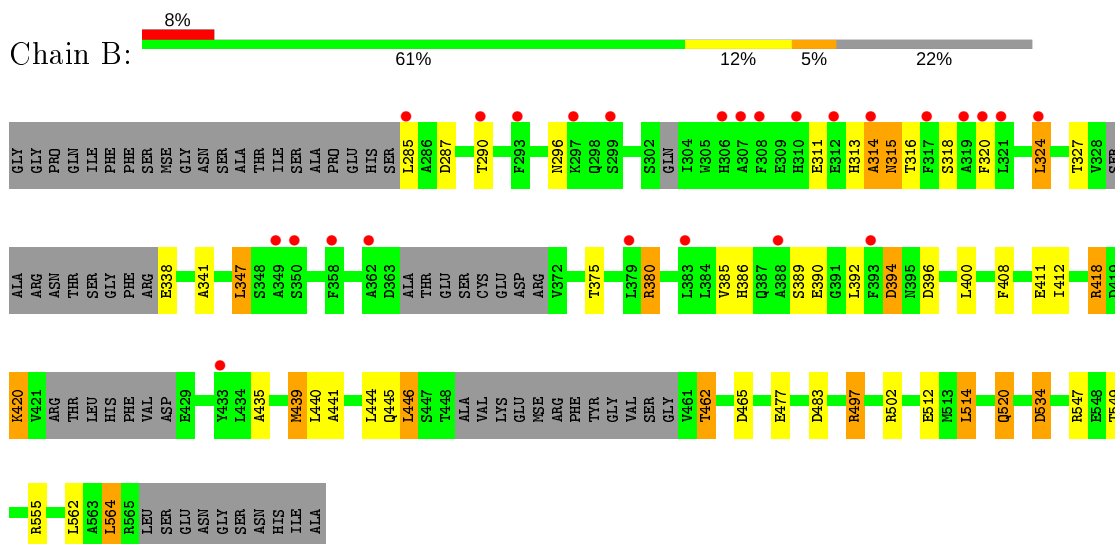
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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: Invasion plasmid antigen, secreted by the Mxi-Spa secretion machinery

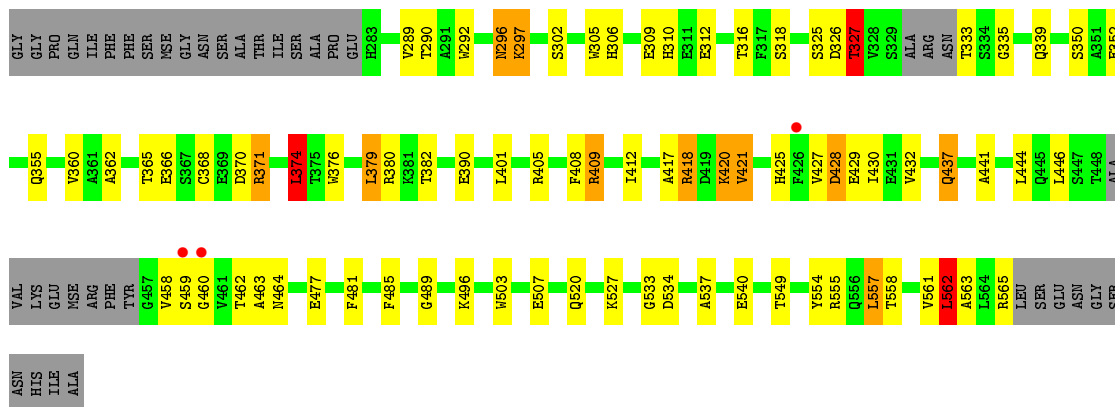


- Molecule 1: Invasion plasmid antigen, secreted by the Mxi-Spa secretion machinery



- Molecule 1: Invasion plasmid antigen, secreted by the Mxi-Spa secretion machinery





4 Data and refinement statistics

Property	Value	Source
Space group	I 4 2 2	Depositor
Cell constants a, b, c, α , β , γ	128.93Å 128.93Å 282.82Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.21 – 2.65 49.19 – 2.65	Depositor EDS
% Data completeness (in resolution range)	99.0 (49.21-2.65) 98.9 (49.19-2.65)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.49 (at 2.65Å)	Xtrriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.228 , 0.284 0.260 , 0.309	Depositor DCC
R_{free} test set	1743 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	58.5	Xtrriage
Anisotropy	0.005	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 49.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	6327	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.44% 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 i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, PEG, 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	0.65	0/2145	0.72	1/2889 (0.0%)
1	B	0.71	0/1996	0.75	3/2688 (0.1%)
1	C	1.04	7/2217 (0.3%)	0.97	8/2990 (0.3%)
All	All	0.83	7/6358 (0.1%)	0.82	12/8567 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	2

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	481	PHE	CE1-CZ	5.96	1.48	1.37
1	C	507	GLU	CG-CD	5.52	1.60	1.51
1	C	485	PHE	CE1-CZ	5.36	1.47	1.37
1	C	390	GLU	CB-CG	-5.33	1.42	1.52
1	C	540	GLU	CG-CD	5.30	1.59	1.51
1	C	376	TRP	CE3-CZ3	5.12	1.47	1.38
1	C	563	ALA	CA-CB	5.08	1.63	1.52

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	409	ARG	NE-CZ-NH2	-8.23	116.19	120.30
1	C	565	ARG	NE-CZ-NH2	-7.70	116.45	120.30
1	C	409	ARG	NE-CZ-NH1	7.14	123.87	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	418	ARG	NE-CZ-NH1	6.39	123.49	120.30
1	C	374	LEU	CA-CB-CG	6.03	129.17	115.30
1	C	565	ARG	NE-CZ-NH1	5.95	123.27	120.30
1	B	347	LEU	CA-CB-CG	5.91	128.89	115.30
1	C	555	ARG	NE-CZ-NH2	5.19	122.90	120.30
1	B	418	ARG	NE-CZ-NH1	5.18	122.89	120.30
1	C	562	LEU	CB-CG-CD2	5.10	119.68	111.00
1	A	483	ASP	CB-CG-OD1	5.08	122.87	118.30
1	B	483	ASP	CB-CG-OD2	-5.02	113.78	118.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	368	CYS	Peptide
1	C	533	GLY	Peptide

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	2114	0	2017	64	0
1	B	1970	0	1885	26	0
1	C	2184	0	2081	41	0
2	B	5	0	0	0	0
2	C	5	0	0	0	0
3	C	18	0	24	1	0
4	C	7	0	10	1	0
5	A	1	0	0	0	0
5	B	4	0	0	0	0
5	C	19	0	0	0	0
All	All	6327	0	6017	130	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 11.

All (130) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:555:ARG:CG	1:A:555:ARG:HH11	1.56	1.16
1:A:555:ARG:HH11	1:A:555:ARG:HG3	1.08	1.11
1:A:303:GLN:HE21	1:A:304:ILE:HG13	1.19	1.06
1:A:555:ARG:NH1	1:A:555:ARG:HG3	1.71	0.97
1:A:468:THR:HG22	1:A:472:MSE:HE2	1.54	0.89
1:B:418:ARG:HH11	1:B:418:ARG:HG2	1.43	0.83
1:B:514:LEU:HD13	1:B:549:THR:HG21	1.61	0.83
1:C:409:ARG:HD3	1:C:477:GLU:OE2	1.80	0.82
1:A:497:ARG:HH11	1:A:497:ARG:CG	1.96	0.78
1:A:555:ARG:HH11	1:A:555:ARG:HG2	1.47	0.78
1:A:497:ARG:HG2	1:A:497:ARG:HH11	1.49	0.77
1:A:541:ALA:HA	1:A:544:GLN:HE21	1.49	0.76
1:A:303:GLN:NE2	1:A:304:ILE:HG13	1.99	0.75
1:C:401:LEU:HD13	4:C:605:PEG:H31	1.71	0.73
1:A:555:ARG:NH1	1:A:555:ARG:CG	2.28	0.72
1:A:409:ARG:HD3	1:A:477:GLU:OE1	1.91	0.71
1:C:417:ALA:HB1	1:C:432:VAL:HG23	1.75	0.68
1:C:405:ARG:O	1:C:409:ARG:HG3	1.94	0.67
1:A:545:VAL:O	1:A:549:THR:HG23	1.96	0.66
1:A:292:TRP:CZ2	1:A:325:SER:HB3	2.30	0.65
1:A:303:GLN:HE21	1:A:304:ILE:CG1	2.03	0.65
1:C:462:THR:HG22	1:C:463:ALA:N	2.10	0.65
1:C:371:ARG:HD3	1:C:374:LEU:HD12	1.79	0.64
1:A:397:THR:HG21	1:A:565:ARG:HH21	1.61	0.63
1:B:420:LYS:O	1:B:420:LYS:HD3	1.98	0.63
1:A:468:THR:CG2	1:A:472:MSE:HE2	2.26	0.63
1:B:502:ARG:NH2	1:B:564:LEU:HD11	2.14	0.62
1:C:458:VAL:HG12	1:C:459:SER:O	1.99	0.62
1:A:405:ARG:O	1:A:409:ARG:HG3	2.00	0.61
1:A:369:GLU:C	1:A:371:ARG:H	2.03	0.61
1:B:514:LEU:CD1	1:B:549:THR:HG21	2.31	0.60
1:C:335:GLY:O	1:C:339:GLN:HG2	2.02	0.60
1:A:497:ARG:CG	1:A:497:ARG:NH1	2.59	0.59
1:C:408:PHE:CE2	1:C:412:ILE:HD11	2.37	0.59
1:A:312:GLU:O	1:A:313:HIS:HB2	2.02	0.59
1:A:369:GLU:O	1:A:371:ARG:N	2.32	0.58
1:A:500:ALA:O	1:A:503:TRP:HB3	2.03	0.58
1:C:558:THR:HG22	1:C:562:LEU:HD22	1.84	0.58
1:C:428:ASP:HB2	1:C:430:ILE:HG22	1.86	0.58
1:A:482:THR:HG22	1:A:555:ARG:HH12	1.69	0.58
1:C:534:ASP:HB3	1:C:537:ALA:HB3	1.85	0.58
1:B:441:ALA:HA	1:B:446:LEU:HB2	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:541:ALA:HA	1:A:544:GLN:NE2	2.19	0.57
1:C:371:ARG:HB3	1:C:418:ARG:HH12	1.68	0.57
1:A:488:TRP:CZ2	1:A:490:PRO:HG2	2.40	0.57
1:C:292:TRP:CZ2	1:C:325:SER:HB3	2.40	0.57
1:A:482:THR:CG2	1:A:555:ARG:HH12	2.18	0.56
1:B:386:HIS:O	1:B:390:GLU:HG2	2.05	0.56
1:C:496:LYS:HE3	1:C:503:TRP:CZ2	2.40	0.56
1:C:421:VAL:HG11	1:C:429:GLU:HA	1.87	0.56
1:B:435:ALA:O	1:B:439:MSE:HG2	2.06	0.55
1:A:482:THR:HB	1:A:555:ARG:HH22	1.72	0.55
1:C:420:LYS:NZ	1:C:460:GLY:O	2.36	0.54
1:A:510:LYS:CB	1:A:553:ILE:HG13	2.37	0.54
1:B:462:THR:HG23	1:B:465:ASP:H	1.72	0.54
1:A:505:GLN:O	1:A:509:GLN:HB2	2.07	0.54
1:B:408:PHE:CZ	1:B:412:ILE:HD11	2.44	0.52
1:A:443:LYS:O	1:A:474:ARG:NH2	2.43	0.52
1:C:325:SER:C	1:C:327:THR:H	2.13	0.52
1:A:347:LEU:HD12	1:A:353:LEU:HD13	1.91	0.51
1:C:296:ASN:ND2	1:C:297:LYS:HG2	2.24	0.51
1:A:468:THR:HG22	1:A:472:MSE:CE	2.32	0.51
1:C:462:THR:HG22	1:C:464:ASN:H	1.76	0.51
1:B:408:PHE:HE2	1:B:477:GLU:HA	1.76	0.50
1:C:316:THR:HG21	1:C:362:ALA:HA	1.92	0.50
1:A:486:SER:OG	1:A:555:ARG:HA	2.11	0.50
1:A:534:ASP:OD1	1:A:534:ASP:C	2.49	0.50
1:A:289:VAL:HG11	1:A:305:TRP:CD2	2.47	0.50
1:A:285:LEU:HD22	1:A:314:ALA:HB1	1.93	0.50
1:B:338:GLU:O	1:B:341:ALA:HB3	2.12	0.49
1:B:408:PHE:CE2	1:B:412:ILE:HD11	2.48	0.49
1:A:434:LEU:HD23	1:A:437:GLN:NE2	2.27	0.49
1:A:365:THR:HG23	1:A:365:THR:O	2.13	0.49
1:A:408:PHE:CZ	1:A:412:ILE:HD11	2.47	0.48
1:B:418:ARG:HH11	1:B:418:ARG:CG	2.20	0.48
1:C:437:GLN:HG2	1:C:446:LEU:HD23	1.95	0.48
1:C:370:ASP:O	1:C:371:ARG:HG3	2.13	0.48
1:B:520:GLN:HE21	1:B:520:GLN:H	1.62	0.48
1:A:534:ASP:O	1:A:538:GLU:HG3	2.14	0.48
1:B:385:VAL:O	1:B:389:SER:HB2	2.14	0.48
1:C:462:THR:CG2	1:C:463:ALA:N	2.77	0.48
1:A:294:PRO:HG2	1:A:296:ASN:HB3	1.96	0.47
1:A:428:ASP:N	1:A:431:GLU:OE2	2.46	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:510:LYS:HB3	1:A:553:ILE:HG13	1.95	0.47
1:A:312:GLU:O	1:A:313:HIS:CB	2.63	0.47
1:C:296:ASN:HD22	1:C:297:LYS:HG2	1.79	0.47
1:A:321:LEU:O	1:A:322:ASP:C	2.53	0.46
1:C:421:VAL:HG11	1:C:429:GLU:CA	2.46	0.45
1:C:350:SER:HA	3:C:603:GOL:H2	1.99	0.45
1:C:462:THR:HG22	1:C:463:ALA:H	1.79	0.45
1:B:394:ASP:OD2	1:B:497:ARG:HD2	2.17	0.45
1:C:302:SER:O	1:C:306:HIS:HB2	2.17	0.45
1:B:285:LEU:CD1	1:B:314:ALA:HB1	2.47	0.44
1:A:488:TRP:CE2	1:A:490:PRO:HG2	2.53	0.43
1:A:366:GLU:CD	1:C:425:HIS:ND1	2.72	0.43
1:A:561:VAL:HA	1:A:564:LEU:CD1	2.48	0.43
1:B:313:HIS:O	1:B:315:ASN:N	2.52	0.43
1:B:408:PHE:CE2	1:B:477:GLU:HA	2.53	0.43
1:A:304:ILE:O	1:A:307:ALA:HB3	2.19	0.43
1:A:294:PRO:HA	1:A:337:ARG:HH22	1.83	0.43
1:A:476:ARG:HG2	1:A:480:GLU:OE1	2.18	0.43
1:C:441:ALA:HA	1:C:446:LEU:HB2	2.00	0.43
1:C:371:ARG:CD	1:C:374:LEU:HD12	2.48	0.43
1:B:420:LYS:C	1:B:420:LYS:HD3	2.38	0.43
1:A:352:GLU:O	1:A:355:GLN:HG3	2.19	0.43
1:A:469:ALA:O	1:A:473:VAL:HG23	2.19	0.42
1:C:289:VAL:HG21	1:C:305:TRP:CE3	2.54	0.42
1:B:439:MSE:H	1:B:439:MSE:HG2	1.43	0.42
1:A:488:TRP:CG	1:A:490:PRO:HD2	2.54	0.42
1:B:320:PHE:CZ	1:B:324:LEU:HD12	2.54	0.42
1:C:444:LEU:HD23	1:C:444:LEU:HA	1.89	0.42
1:C:558:THR:CG2	1:C:562:LEU:HD22	2.47	0.42
1:A:549:THR:O	1:A:553:ILE:HG12	2.20	0.42
1:B:440:LEU:HB3	1:B:444:LEU:HD12	2.00	0.42
1:C:296:ASN:HD22	1:C:297:LYS:NZ	2.18	0.42
1:B:380:ARG:HH11	1:B:380:ARG:HG2	1.85	0.41
1:B:534:ASP:OD1	1:B:534:ASP:C	2.57	0.41
1:C:554:TYR:HA	1:C:554:TYR:HD1	1.74	0.41
1:C:557:LEU:O	1:C:561:VAL:HG23	2.20	0.41
1:C:360:VAL:HG21	1:C:382:THR:OG1	2.20	0.41
1:A:290:THR:C	1:A:292:TRP:H	2.24	0.41
1:C:421:VAL:HG11	1:C:429:GLU:N	2.35	0.41
1:A:295:GLU:H	1:A:295:GLU:CD	2.23	0.41
1:A:356:GLN:O	1:A:360:VAL:HG23	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:555:ARG:NH1	1:A:555:ARG:HG2	2.20	0.41
1:A:369:GLU:C	1:A:371:ARG:N	2.72	0.40
1:A:497:ARG:HG3	1:A:497:ARG:NH1	2.33	0.40
1:C:360:VAL:CG1	1:C:379:LEU:HD13	2.51	0.40
1:A:495:LEU:HD13	1:A:557:LEU:CD1	2.51	0.40
1:A:561:VAL:HA	1:A:564:LEU:HD12	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	254/312 (81%)	219 (86%)	31 (12%)	4 (2%)	9	14
1	B	232/312 (74%)	207 (89%)	20 (9%)	5 (2%)	6	9
1	C	266/312 (85%)	247 (93%)	16 (6%)	3 (1%)	14	21
All	All	752/936 (80%)	673 (90%)	67 (9%)	12 (2%)	9	14

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	313	HIS
1	B	394	ASP
1	A	370	ASP
1	B	314	ALA
1	B	564	LEU
1	C	327	THR
1	A	296	ASN
1	A	326	ASP
1	B	311	GLU
1	C	326	ASP
1	B	396	ASP

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Mol	Chain	Res	Type
1	C	489	GLY

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	218/252 (86%)	183 (84%)	35 (16%)	2	2
1	B	204/252 (81%)	177 (87%)	27 (13%)	4	5
1	C	228/252 (90%)	201 (88%)	27 (12%)	5	7
All	All	650/756 (86%)	561 (86%)	89 (14%)	3	4

All (89) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	290	THR
1	A	295	GLU
1	A	310	HIS
1	A	327	THR
1	A	338	GLU
1	A	352	GLU
1	A	353	LEU
1	A	355	GLN
1	A	356	GLN
1	A	363	ASP
1	A	366	GLU
1	A	367	SER
1	A	384	LEU
1	A	392	LEU
1	A	397	THR
1	A	400	LEU
1	A	414	GLU
1	A	418	ARG
1	A	419	ASP
1	A	421	VAL
1	A	428	ASP

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Mol	Chain	Res	Type
1	A	439	MSE
1	A	446	LEU
1	A	487	LEU
1	A	497	ARG
1	A	509	GLN
1	A	510	LYS
1	A	514	LEU
1	A	527	LYS
1	A	539	ARG
1	A	549	THR
1	A	555	ARG
1	A	557	LEU
1	A	564	LEU
1	A	565	ARG
1	B	287	ASP
1	B	290	THR
1	B	296	ASN
1	B	315	ASN
1	B	316	THR
1	B	318	SER
1	B	324	LEU
1	B	327	THR
1	B	347	LEU
1	B	375	THR
1	B	380	ARG
1	B	392	LEU
1	B	400	LEU
1	B	411	GLU
1	B	420	LYS
1	B	439	MSE
1	B	445	GLN
1	B	446	LEU
1	B	462	THR
1	B	497	ARG
1	B	512	GLU
1	B	514	LEU
1	B	520	GLN
1	B	534	ASP
1	B	547	ARG
1	B	555	ARG
1	B	562	LEU
1	C	290	THR

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Mol	Chain	Res	Type
1	C	296	ASN
1	C	297	LYS
1	C	309	GLU
1	C	310	HIS
1	C	312	GLU
1	C	318	SER
1	C	327	THR
1	C	333	THR
1	C	352	GLU
1	C	355	GLN
1	C	365	THR
1	C	366	GLU
1	C	371	ARG
1	C	374	LEU
1	C	379	LEU
1	C	380	ARG
1	C	420	LYS
1	C	421	VAL
1	C	427	VAL
1	C	428	ASP
1	C	437	GLN
1	C	520	GLN
1	C	527	LYS
1	C	549	THR
1	C	557	LEU
1	C	562	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	303	GLN
1	A	377	ASN
1	A	378	ASN
1	A	437	GLN
1	A	516	ASN
1	A	544	GLN
1	B	296	ASN
1	B	395	ASN
1	B	437	GLN
1	B	520	GLN
1	C	283	HIS
1	C	296	ASN

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Mol	Chain	Res	Type
1	C	437	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

6 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	PEG	C	605	-	6,6,6	0.65	0	5,5,5	0.56	0
2	SO4	C	600	-	4,4,4	0.14	0	6,6,6	0.61	0
3	GOL	C	602	-	5,5,5	0.41	0	5,5,5	0.58	0
3	GOL	C	604	-	5,5,5	0.26	0	5,5,5	0.80	0
2	SO4	B	601	-	4,4,4	0.16	0	6,6,6	0.30	0
3	GOL	C	603	-	5,5,5	0.43	0	5,5,5	0.42	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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PEG	C	605	-	-	1/4/4/4	-
3	GOL	C	604	-	-	4/4/4/4	-
3	GOL	C	603	-	-	1/4/4/4	-
3	GOL	C	602	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	602	GOL	C1-C2-C3-O3
3	C	604	GOL	O1-C1-C2-C3
3	C	604	GOL	C1-C2-C3-O3
4	C	605	PEG	O1-C1-C2-O2
3	C	602	GOL	O2-C2-C3-O3
3	C	604	GOL	O2-C2-C3-O3
3	C	604	GOL	O1-C1-C2-O2
3	C	603	GOL	C1-C2-C3-O3

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	605	PEG	1	0
3	C	603	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	257/312 (82%)	0.74	21 (8%) 11 9	63, 81, 105, 113	22 (8%)
1	B	239/312 (76%)	0.69	25 (10%) 6 4	46, 62, 81, 89	9 (3%)
1	C	267/312 (85%)	0.16	3 (1%) 80 79	24, 36, 67, 79	9 (3%)
All	All	763/936 (81%)	0.52	49 (6%) 19 16	24, 63, 93, 113	40 (5%)

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	395	ASN	4.9
1	A	305	TRP	4.7
1	A	293	PHE	4.6
1	B	285	LEU	4.1
1	B	350	SER	4.1
1	B	320	PHE	4.0
1	B	290	THR	3.9
1	B	319	ALA	3.9
1	A	537	ALA	3.7
1	B	314	ALA	3.7
1	B	349	ALA	3.7
1	B	299	SER	3.7
1	B	321	LEU	3.6
1	B	310	HIS	3.6
1	B	308	PHE	3.6
1	B	307	ALA	3.6
1	A	422	ARG	3.5
1	A	304	ILE	3.5
1	C	460	GLY	3.4
1	A	324	LEU	2.9
1	B	379	LEU	2.9
1	A	289	VAL	2.8
1	B	358	PHE	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	459	SER	2.7
1	B	388	ALA	2.6
1	B	293	PHE	2.6
1	A	306	HIS	2.6
1	A	321	LEU	2.6
1	B	433	TYR	2.6
1	B	297	LYS	2.6
1	B	393	PHE	2.5
1	C	426	PHE	2.5
1	A	335	GLY	2.4
1	A	290	THR	2.4
1	B	362	ALA	2.3
1	A	562	LEU	2.3
1	A	294	PRO	2.3
1	A	533	GLY	2.2
1	B	317	PHE	2.2
1	A	401	LEU	2.1
1	A	303	GLN	2.1
1	B	383	LEU	2.1
1	A	320	PHE	2.1
1	A	418	ARG	2.1
1	B	324	LEU	2.1
1	A	322	ASP	2.0
1	A	532	SER	2.0
1	B	306	HIS	2.0
1	B	312	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 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. 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(\AA^2)	Q<0.9
4	PEG	C	605	7/7	0.87	0.21	43,52,61,64	0
3	GOL	C	603	6/6	0.89	0.22	49,53,54,55	6
3	GOL	C	604	6/6	0.90	0.18	63,65,67,72	0
3	GOL	C	602	6/6	0.91	0.26	44,46,46,47	6
2	SO4	B	601	5/5	0.96	0.16	55,56,58,59	5
2	SO4	C	600	5/5	0.98	0.11	48,48,51,51	5

6.5 Other polymers [i](#)

There are no such residues in this entry.