



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 10:53 AM UTC

PDB ID : 3CKD / pdb_00003ckd
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 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

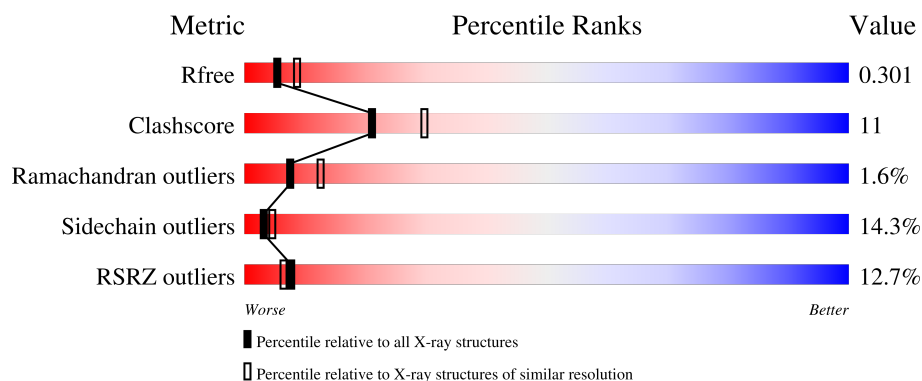
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.65 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}	180053	1110 (2.66-2.66)
Clashscore	190562	1141 (2.66-2.66)
Ramachandran outliers	187476	1126 (2.66-2.66)
Sidechain outliers	187428	1126 (2.66-2.66)
RSRZ outliers	180081	1110 (2.66-2.66)

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	312	19% 54% 23% 7% 16%
1	B	312	9% 61% 13% 5% 22%
1	C	312	4% 60% 23% • 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
1	A	262	Total	C	N	O	S	Se	0	0	0
			2114	1319	373	416	1	5			
1	B	244	Total	C	N	O	Se		0	0	0
			1970	1233	343	389	5				
1	C	272	Total	C	N	O	S	Se	0	0	0
			2184	1359	385	434	1	5			

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 (CCD ID: SO4) (formula: O₄S).



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

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 4 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



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

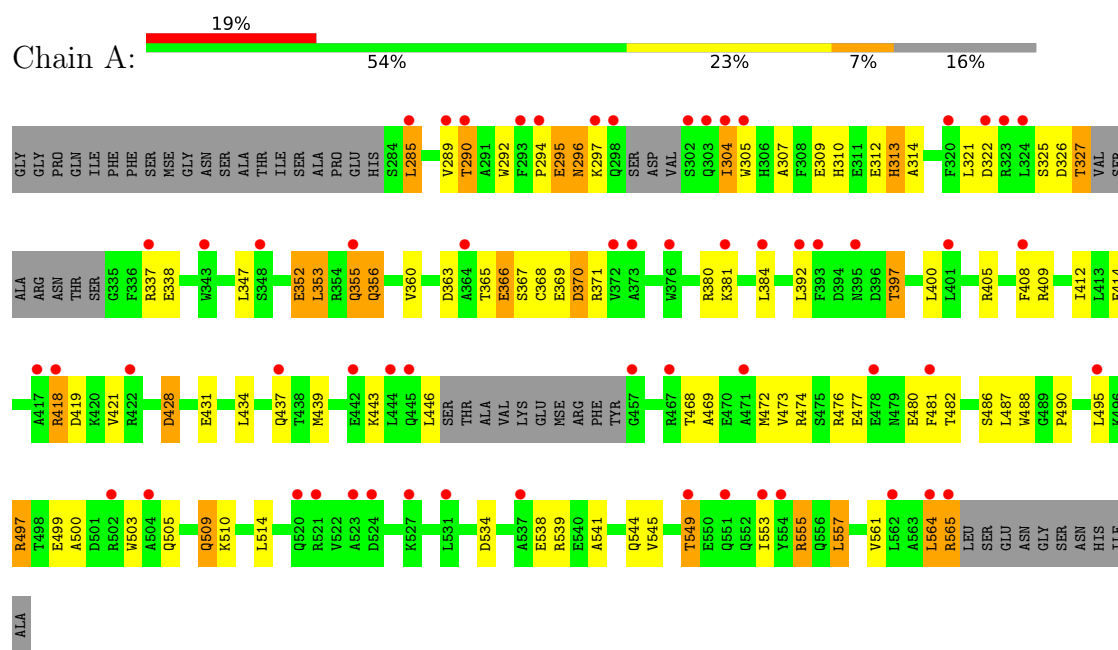
- Molecule 5 is water.

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

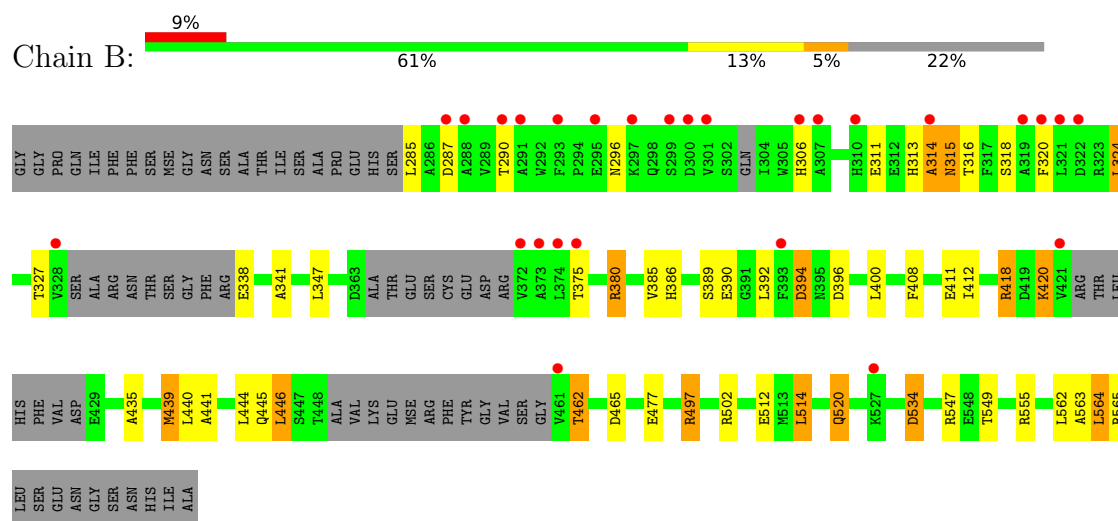
3 Residue-property plots [i](#)

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.

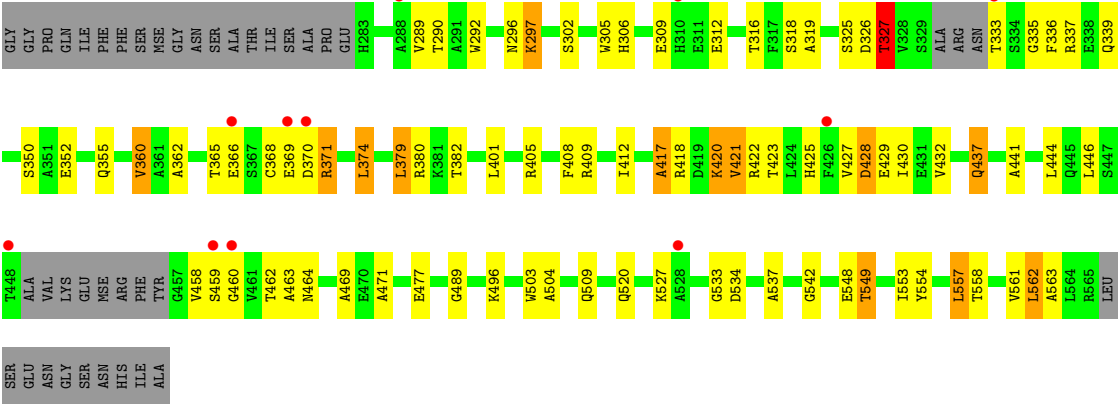
- Molecule 1: Invasion plasmid antigen, secreted by the Mxi-Spa secretion machinery



- 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 49.21 – 2.65	Depositor EDS
% Data completeness (in resolution range)	99.0 (49.21-2.65) 98.9 (49.21-2.65)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.49 (at 2.65Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.228 , 0.284 (Not available) , 0.301	Depositor DCC
R_{free} test set	1743 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	58.5	Xtriage
Anisotropy	0.005	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 46.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
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

Xtriage'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 ⓘ

5.1 Standard geometry ⓘ

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	0.79	0/2145	0.98	1/2889 (0.0%)
1	B	0.83	0/1996	1.00	0/2688
1	C	1.21	7/2217 (0.3%)	1.18	6/2990 (0.2%)
All	All	0.97	7/6358 (0.1%)	1.06	7/8567 (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	563	ALA	CA-CB	5.76	1.63	1.53
1	C	504	ALA	CA-CB	5.43	1.61	1.53
1	C	542	GLY	C-O	5.37	1.30	1.23
1	C	319	ALA	CA-CB	-5.35	1.45	1.53
1	C	417	ALA	CA-CB	-5.15	1.45	1.53
1	C	471	ALA	CA-CB	-5.06	1.45	1.53
1	C	360	VAL	CA-CB	5.03	1.60	1.54

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	469	ALA	N-CA-C	-5.83	104.84	111.14
1	C	548	GLU	CA-C-N	-5.42	112.60	120.29
1	C	548	GLU	C-N-CA	-5.42	112.60	120.29

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	369	GLU	N-CA-C	-5.30	102.62	110.46
1	C	549	THR	N-CA-CB	5.27	117.96	110.16
1	A	418	ARG	N-CA-C	-5.16	105.55	111.07
1	C	553	ILE	CB-CA-C	-5.10	105.44	111.97

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	66	0
1	B	1970	0	1885	27	0
1	C	2184	0	2081	43	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	135	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 (135) 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:HH11	1:A:555:ARG:CG	1.56	1.16

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:555:ARG:HH11	1:A:555:ARG:HG3	1.08	1.11
1:A:555:ARG:HG3	1:A:555:ARG:NH1	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:CG	1:A:497:ARG:HH11	1.96	0.78
1:A:555:ARG:HH11	1:A:555:ARG:HG2	1.47	0.78
1:A:497:ARG:HH11	1:A:497:ARG:HG2	1.49	0.77
1:A:541:ALA:HA	1:A:544:GLN:HE21	1.49	0.76
1:C:401:LEU:HD13	4:C:605:PEG:H31	1.71	0.73
1:A:555:ARG:CG	1:A:555:ARG:NH1	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:369:GLU:C	1:A:371:ARG:H	2.03	0.66
1:A:292:TRP:CZ2	1:A:325:SER:HB3	2.30	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: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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:325:SER:C	1:C:327:THR:H	2.13	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:534:ASP:OD1	1:A:534:ASP:C	2.49	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: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:321:LEU:O	1:A:322:ASP:C	2.53	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: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:O	1:A:365:THR:HG23	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:A:366:GLU:CD	1:C:425:HIS:ND1	2.72	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:B:420:LYS:HD3	1:B:420:LYS:C	2.38	0.47
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

Continued on next page...

Continued from previous page...

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:B:534:ASP:OD1	1:B:534:ASP:C	2.57	0.46
1:A:290:THR:C	1:A:292:TRP:H	2.24	0.46
1:A:369:GLU:C	1:A:371:ARG:N	2.72	0.46
1:A:295:GLU:H	1:A:295:GLU:CD	2.23	0.46
1:C:350:SER:HA	3:C:603:GOL:H2	1.99	0.45
1:C:421:VAL:HG11	1:C:429:GLU:CA	2.46	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:A:368:CYS:C	1:A:370:ASP:H	2.24	0.45
1:B:285:LEU:CD1	1:B:314:ALA:HB1	2.47	0.44
1:C:336:PHE:O	1:C:337:ARG:C	2.59	0.44
1:A:488:TRP:CE2	1:A:490:PRO:HG2	2.53	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:A:352:GLU:O	1:A:355:GLN:HG3	2.19	0.43
1:A:325:SER:C	1:A:327:THR:H	2.26	0.42
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:HG2	1:B:439:MSE:H	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:A:380:ARG:O	1:A:381:LYS:C	2.63	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:C:554:TYR:HD1	1:C:554:TYR:HA	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:421:VAL:HG11	1:C:429:GLU:N	2.35	0.41
1:A:290:THR:C	1:A:292:TRP:N	2.78	0.41
1:A:481:PHE:O	1:A:482:THR:C	2.64	0.41
1:B:563:ALA:C	1:B:565:ARG:H	2.29	0.41
1:A:356:GLN:O	1:A:360:VAL:HG23	2.20	0.41
1:A:555:ARG:NH1	1:A:555:ARG:HG2	2.20	0.41
1:C:422:ARG:O	1:C:423:THR:C	2.63	0.40
1:A:497:ARG:NH1	1:A:497:ARG:HG3	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%)	7	12
1	B	232/312 (74%)	207 (89%)	20 (9%)	5 (2%)	5	9
1	C	266/312 (85%)	247 (93%)	16 (6%)	3 (1%)	11	19
All	All	752/936 (80%)	673 (90%)	67 (9%)	12 (2%)	7	12

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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	296	ASN
1	A	326	ASP
1	B	311	GLU
1	C	326	ASP
1	B	396	ASP
1	C	489	GLY

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	218/252 (86%)	180 (83%)	38 (17%)	2	2
1	B	204/252 (81%)	175 (86%)	29 (14%)	3	5
1	C	228/252 (90%)	202 (89%)	26 (11%)	5	8
All	All	650/756 (86%)	557 (86%)	93 (14%)	3	4

All (93) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	285	LEU
1	A	290	THR
1	A	295	GLU
1	A	297	LYS
1	A	304	ILE
1	A	309	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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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
1	A	439	MSE
1	A	446	LEU
1	A	487	LEU
1	A	497	ARG
1	A	499	GLU
1	A	509	GLN
1	A	514	LEU
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	306	HIS
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	418	ARG
1	B	420	LYS
1	B	439	MSE
1	B	445	GLN
1	B	446	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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
1	C	297	LYS
1	C	309	GLU
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	509	GLN
1	C	520	GLN
1	C	527	LYS
1	C	549	THR
1	C	557	LEU
1	C	562	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	303	GLN
1	A	306	HIS
1	A	356	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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	356	GLN
1	B	378	ASN
1	B	387	GLN
1	B	395	ASN
1	B	509	GLN
1	B	520	GLN
1	C	283	HIS
1	C	296	ASN
1	C	387	GLN
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 oligosaccharides 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
3	GOL	C	603	-	5,5,5	0.45	0	5,5,5	0.43	0
3	GOL	C	602	-	5,5,5	0.42	0	5,5,5	0.63	0
2	SO4	B	601	-	4,4,4	0.22	0	6,6,6	0.29	0
2	SO4	C	600	-	4,4,4	0.23	0	6,6,6	0.58	0
3	GOL	C	604	-	5,5,5	0.26	0	5,5,5	0.86	0
4	PEG	C	605	-	6,6,6	0.66	0	5,5,5	0.56	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
4	PEG	C	605	-	-	1/4/4/4	-
3	GOL	C	603	-	-	0/4/4/4	-
3	GOL	C	604	-	-	4/4/4/4	-
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 (7) 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

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	603	GOL	1	0
4	C	605	PEG	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%)	1.55	59 (22%) 2 1	55, 79, 105, 113	22 (8%)
1	B	239/312 (76%)	0.79	27 (11%) 10 8	40, 61, 80, 88	9 (3%)
1	C	267/312 (85%)	0.15	11 (4%) 41 33	24, 36, 66, 79	9 (3%)
All	All	763/936 (81%)	0.82	97 (12%) 8 6	24, 62, 92, 113	40 (5%)

All (97) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	372	VAL	8.3
1	A	304	ILE	6.3
1	A	395	ASN	6.2
1	A	293	PHE	5.7
1	B	290	THR	5.5
1	A	527	LYS	5.2
1	A	320	PHE	4.7
1	A	502	ARG	4.7
1	A	445	GLN	4.7
1	A	305	TRP	4.4
1	A	303	GLN	4.3
1	B	328	VAL	4.1
1	B	461	VAL	3.9
1	C	459	SER	3.9
1	A	521	ARG	3.8
1	A	302	SER	3.8
1	A	562	LEU	3.7
1	B	291	ALA	3.7
1	A	290	THR	3.7
1	A	551	GLN	3.7
1	B	374	LEU	3.6
1	A	442	GLU	3.6
1	A	324	LEU	3.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	297	LYS	3.5
1	A	355	GLN	3.4
1	B	306	HIS	3.4
1	B	373	ALA	3.4
1	B	299	SER	3.3
1	A	549	THR	3.3
1	A	422	ARG	3.3
1	A	372	VAL	3.3
1	C	448	THR	3.2
1	C	369	GLU	3.1
1	B	375	THR	3.1
1	A	376	TRP	3.0
1	A	564	LEU	3.0
1	A	401	LEU	2.9
1	A	348	SER	2.9
1	A	554	TYR	2.9
1	A	457	GLY	2.8
1	B	320	PHE	2.8
1	B	307	ALA	2.8
1	A	408	PHE	2.6
1	B	322	ASP	2.6
1	B	319	ALA	2.6
1	A	531	LEU	2.6
1	A	444	LEU	2.6
1	C	460	GLY	2.6
1	C	426	PHE	2.6
1	A	337	ARG	2.5
1	A	381	LYS	2.5
1	A	418	ARG	2.5
1	A	553	ILE	2.5
1	A	392	LEU	2.5
1	B	287	ASP	2.5
1	B	321	LEU	2.5
1	A	504	ALA	2.4
1	A	524	ASP	2.4
1	A	393	PHE	2.4
1	B	293	PHE	2.4
1	C	528	ALA	2.4
1	C	288	ALA	2.4
1	A	298	GLN	2.4
1	B	393	PHE	2.4
1	C	310	HIS	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	301	VAL	2.3
1	A	384	LEU	2.3
1	C	333	THR	2.3
1	A	478	GLU	2.3
1	A	495	LEU	2.3
1	C	366	GLU	2.3
1	C	370	ASP	2.3
1	A	285	LEU	2.2
1	A	364	ALA	2.2
1	B	288	ALA	2.2
1	B	297	LYS	2.2
1	B	314	ALA	2.2
1	A	417	ALA	2.2
1	A	537	ALA	2.2
1	A	289	VAL	2.2
1	A	471	ALA	2.1
1	A	323	ARG	2.1
1	A	373	ALA	2.1
1	B	300	ASP	2.1
1	A	523	ALA	2.1
1	A	565	ARG	2.1
1	A	343	TRP	2.1
1	B	527	LYS	2.1
1	A	322	ASP	2.0
1	B	295	GLU	2.0
1	A	520	GLN	2.0
1	A	481	PHE	2.0
1	A	294	PRO	2.0
1	A	437	GLN	2.0
1	B	310	HIS	2.0
1	A	467	ARG	2.0
1	B	421	VAL	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	GOL	C	603	6/6	0.76	0.24	49,53,54,55	6
3	GOL	C	604	6/6	0.76	0.25	63,65,67,72	0
3	GOL	C	602	6/6	0.80	0.25	44,46,46,47	6
4	PEG	C	605	7/7	0.92	0.12	43,52,61,64	0
2	SO4	B	601	5/5	0.95	0.09	55,56,58,59	5
2	SO4	C	600	5/5	0.98	0.04	48,48,51,51	5

6.5 Other polymers [i](#)

There are no such residues in this entry.