



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 08:09 PM UTC

PDB ID : 8T5Q / pdb_00008t5q
Title : SARS-CoV-2 ORF3a peptide in complex with TRAF2 TRAF domain
Authors : Busscher, B.M.; Xiao, T.S.
Deposited on : 2023-06-14
Resolution : 1.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

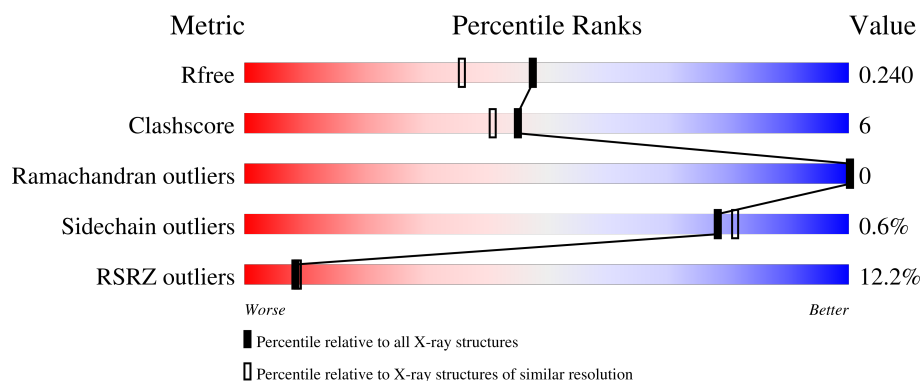
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	188	6% 81% 8% 11%
1	B	188	7% 77% 12% 11%
1	C	188	11% 77% 12% 11%
1	D	188	16% 76% 13% 11%
1	E	188	9% 79% 10% 11%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	188	13% 73% 16% 11%
2	G	5	20% 80% 20%
2	H	5	100% 100%
2	I	5	60% 80% 20%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8505 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 TNF receptor-associated factor 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	168	Total	C	N	O	S	0	0	0
			1334	853	229	242	10			
1	B	168	Total	C	N	O	S	0	0	0
			1334	853	229	242	10			
1	C	168	Total	C	N	O	S	0	0	0
			1334	853	229	242	10			
1	D	168	Total	C	N	O	S	0	0	0
			1334	853	229	242	10			
1	E	168	Total	C	N	O	S	0	0	0
			1334	853	229	242	10			
1	F	168	Total	C	N	O	S	0	0	0
			1334	853	229	242	10			

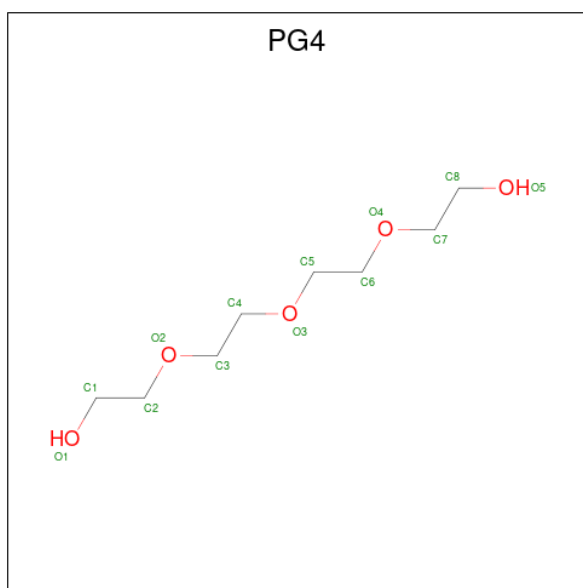
There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	314	SER	-	expression tag	UNP Q12933
B	314	SER	-	expression tag	UNP Q12933
C	314	SER	-	expression tag	UNP Q12933
D	314	SER	-	expression tag	UNP Q12933
E	314	SER	-	expression tag	UNP Q12933
F	314	SER	-	expression tag	UNP Q12933

- Molecule 2 is a protein called ORF3a protein.

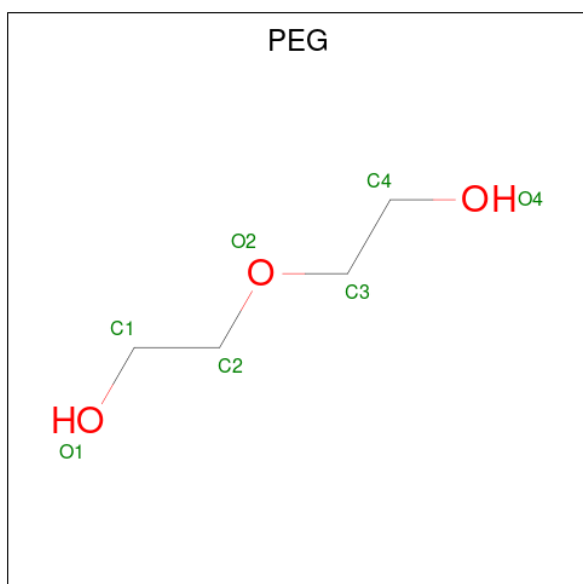
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	G	5	Total	C	N	O	0	0	0
			35	22	6	7			
2	H	5	Total	C	N	O	0	0	0
			35	22	6	7			
2	I	5	Total	C	N	O	1	0	0
			35	22	6	7			

- Molecule 3 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: $C_8H_{18}O_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			13	8	5		
3	B	1	Total	C	O	0	0
			13	8	5		
3	D	1	Total	C	O	0	0
			13	8	5		
3	F	1	Total	C	O	0	0
			13	8	5		

- 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 7 4 3	0	0
4	C	1	Total C O 7 4 3	0	0
4	E	1	Total C O 7 4 3	0	0
4	E	1	Total C O 7 4 3	0	0

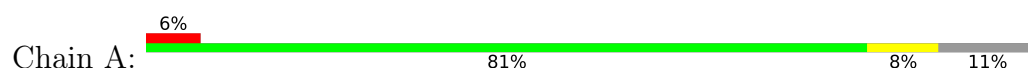
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	65	Total O 65 65	0	0
5	B	60	Total O 60 60	0	0
5	C	61	Total O 61 61	0	0
5	D	27	Total O 27 27	0	0
5	E	67	Total O 67 67	0	0
5	F	34	Total O 34 34	0	0
5	G	1	Total O 1 1	0	0
5	H	1	Total O 1 1	0	0

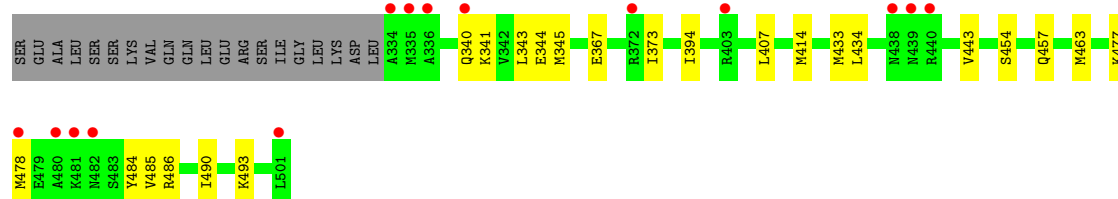
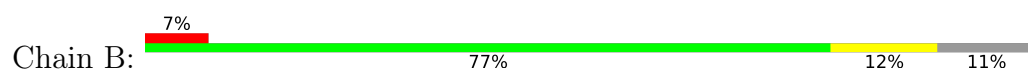
3 Residue-property plots [i](#)

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.

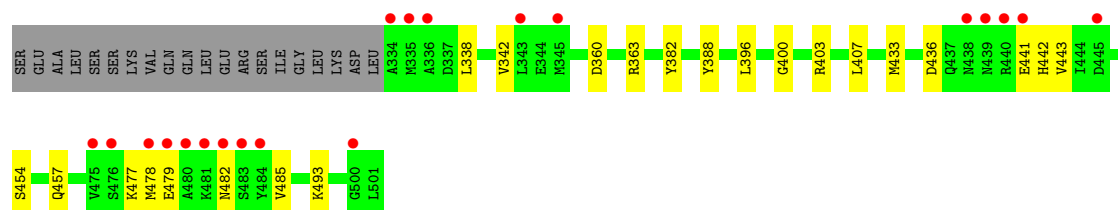
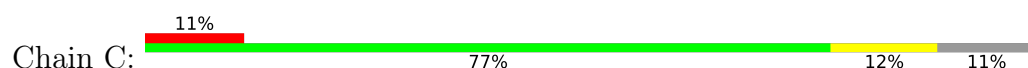
- Molecule 1: TNF receptor-associated factor 2



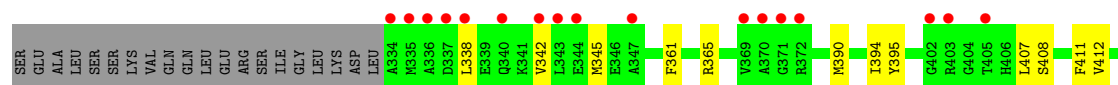
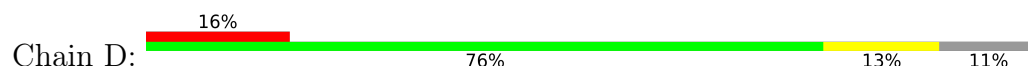
- Molecule 1: TNF receptor-associated factor 2



- Molecule 1: TNF receptor-associated factor 2

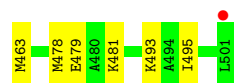
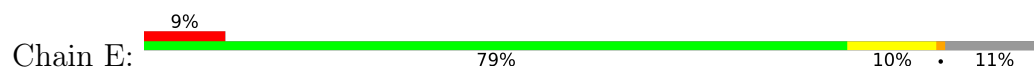


- Molecule 1: TNF receptor-associated factor 2

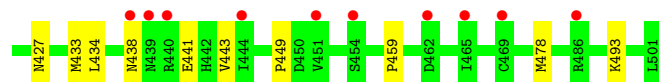
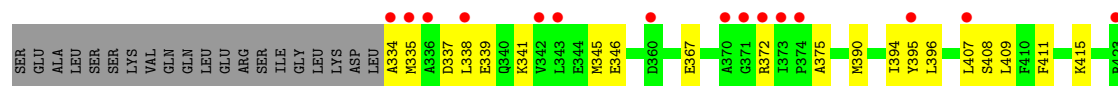




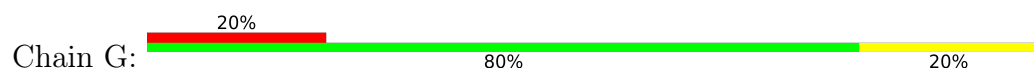
- Molecule 1: TNF receptor-associated factor 2



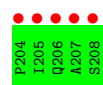
- Molecule 1: TNF receptor-associated factor 2



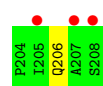
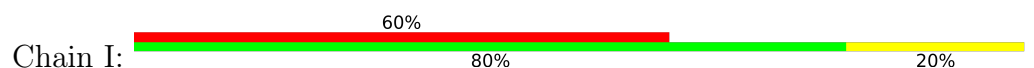
- Molecule 2: ORF3a protein



- Molecule 2: ORF3a protein



- Molecule 2: ORF3a protein



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	135.20Å 84.22Å 124.39Å 90.00° 118.82° 90.00°	Depositor
Resolution (Å)	29.61 – 1.90 29.61 – 1.90	Depositor EDS
% Data completeness (in resolution range)	98.7 (29.61-1.90) 98.8 (29.61-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.56 (at 1.89Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487, PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.207 , 0.240 0.207 , 0.240	Depositor DCC
R_{free} test set	4759 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å ²)	29.6	Xtriage
Anisotropy	0.448	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 40.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	8505	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 29.28 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.5917e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: PEG, PG4

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	0.34	0/1364	0.55	0/1842
1	B	0.35	0/1364	0.58	0/1842
1	C	0.34	0/1364	0.53	0/1842
1	D	0.27	0/1364	0.52	0/1842
1	E	0.38	0/1364	0.57	0/1842
1	F	0.28	0/1364	0.57	0/1842
2	G	0.23	0/35	0.43	0/46
2	H	0.16	0/35	0.31	0/46
2	I	0.19	0/35	0.21	0/46
All	All	0.33	0/8289	0.55	0/11190

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	E	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	365	ARG	Sidechain

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	1334	0	1328	10	0
1	B	1334	0	1328	17	0
1	C	1334	0	1328	23	0
1	D	1334	0	1328	23	0
1	E	1334	0	1328	11	0
1	F	1334	0	1328	22	0
2	G	35	0	36	1	0
2	H	35	0	36	0	0
2	I	35	0	36	1	0
3	A	13	0	18	1	0
3	B	13	0	18	3	0
3	D	13	0	18	0	0
3	F	13	0	18	1	0
4	C	14	0	20	3	0
4	E	14	0	20	0	0
5	A	65	0	0	0	0
5	B	60	0	0	0	0
5	C	61	0	0	0	0
5	D	27	0	0	0	0
5	E	67	0	0	0	0
5	F	34	0	0	0	0
5	G	1	0	0	0	0
5	H	1	0	0	0	0
All	All	8505	0	8188	97	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 6.

All (97) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:407:LEU:HD13	1:C:478:MET:HE1	1.50	0.90
1:B:493:LYS:HZ2	3:B:601:PG4:H61	1.37	0.88
1:C:436:ASP:H	1:C:442:HIS:HD2	1.24	0.85
1:D:345:MET:HE3	1:F:345:MET:HE2	1.61	0.80

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:482:ASN:HD21	1:C:485:VAL:H	1.32	0.78
1:B:486:ARG:HG3	1:B:486:ARG:HH11	1.53	0.73
1:C:479:GLU:H	1:C:482:ASN:HB3	1.57	0.68
1:D:338:LEU:HD21	1:F:338:LEU:HB3	1.77	0.66
1:B:434:LEU:HD21	1:B:478:MET:HE1	1.78	0.65
1:D:338:LEU:HD13	1:F:339:GLU:HG2	1.79	0.65
1:E:393:ARG:NH1	1:E:395:TYR:OH	2.32	0.63
1:F:367:GLU:HG2	1:F:372:ARG:HH12	1.64	0.62
1:D:345:MET:CE	1:F:345:MET:HE2	2.30	0.62
1:F:341:LYS:O	1:F:345:MET:HG2	2.00	0.62
1:E:335:MET:HE1	1:F:335:MET:HG3	1.82	0.61
1:A:345:MET:HE1	1:C:342:VAL:HG13	1.82	0.61
1:D:338:LEU:O	1:D:342:VAL:HG23	2.01	0.61
1:E:479:GLU:OE2	1:E:481:LYS:HE3	2.00	0.60
1:B:341:LYS:O	1:B:345:MET:HG3	2.01	0.59
1:A:353:VAL:HG11	3:A:601:PG4:H21	1.84	0.59
1:F:334:ALA:N	1:F:337:ASP:OD2	2.35	0.59
1:D:395:TYR:HB2	1:D:408:SER:HB2	1.85	0.58
1:F:434:LEU:HD21	1:F:478:MET:HE1	1.84	0.58
1:E:414:MET:HE3	1:E:463:MET:HE2	1.85	0.58
1:B:414:MET:HE3	1:B:463:MET:HE2	1.85	0.57
1:C:441:GLU:OE1	1:C:477:LYS:NZ	2.36	0.57
1:C:400:GLY:H	1:C:403:ARG:NH1	2.03	0.57
1:E:434:LEU:HD21	1:E:478:MET:HE1	1.87	0.55
1:F:395:TYR:HB2	1:F:408:SER:HB2	1.89	0.55
1:C:482:ASN:ND2	1:C:485:VAL:H	2.01	0.55
1:D:394:ILE:HD11	1:D:407:LEU:HD21	1.90	0.54
1:C:436:ASP:N	1:C:442:HIS:HD2	2.01	0.54
1:D:390:MET:HG2	1:D:411:PHE:CZ	2.42	0.54
1:C:478:MET:HA	1:C:482:ASN:HD22	1.73	0.54
1:D:479:GLU:HG3	1:D:480:ALA:N	2.23	0.54
1:C:482:ASN:HD21	1:C:485:VAL:N	2.04	0.52
1:B:486:ARG:HG3	1:B:486:ARG:NH1	2.24	0.51
1:D:479:GLU:HG2	1:D:481:LYS:H	1.75	0.51
1:B:493:LYS:HZ2	3:B:601:PG4:C6	2.17	0.51
1:C:396:LEU:HA	1:C:407:LEU:HD12	1.92	0.50
1:B:478:MET:HA	1:B:478:MET:HE2	1.94	0.50
1:C:396:LEU:HD23	1:C:407:LEU:HD11	1.93	0.50
1:D:407:LEU:N	1:D:473:CYS:O	2.44	0.50
1:A:335:MET:HE2	1:A:335:MET:HA	1.94	0.49
1:B:340:GLN:O	1:B:344:GLU:HG3	2.12	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:415:LYS:HB2	1:D:459:PRO:HB2	1.94	0.49
1:E:425:PRO:HG2	1:E:451:VAL:HG22	1.94	0.49
1:F:415:LYS:HA	1:F:459:PRO:HG2	1.93	0.48
1:F:372:ARG:NH1	1:F:372:ARG:HB3	2.28	0.48
1:D:467:SER:HA	2:I:206:GLN:HA	1.96	0.48
1:D:361:PHE:HZ	1:D:478:MET:HE3	1.79	0.47
1:B:367:GLU:CD	1:B:373:ILE:HD13	2.39	0.47
1:C:478:MET:HA	1:C:482:ASN:ND2	2.29	0.47
1:E:361:PHE:HZ	1:E:478:MET:HG3	1.79	0.47
1:D:407:LEU:HD12	1:D:478:MET:SD	2.55	0.47
1:B:394:ILE:HD11	1:B:407:LEU:HD21	1.95	0.47
1:C:360:ASP:OD2	1:C:363:ARG:NH2	2.24	0.47
1:E:493:LYS:HE2	1:E:495:ILE:HD11	1.97	0.47
1:F:335:MET:O	1:F:339:GLU:HG3	2.13	0.47
1:B:477:LYS:HD3	1:B:484:TYR:CE2	2.50	0.46
1:C:493:LYS:HD3	4:C:602:PEG:H41	1.96	0.46
1:F:394:ILE:HD12	1:F:409:LEU:HD13	1.98	0.46
1:F:427:ASN:HA	1:F:449:PRO:HG2	1.98	0.45
1:F:390:MET:HG2	1:F:411:PHE:CZ	2.51	0.45
1:A:415:LYS:HZ1	1:A:460:VAL:C	2.24	0.45
1:B:493:LYS:NZ	3:B:601:PG4:H61	2.20	0.45
1:D:390:MET:HE3	1:D:390:MET:HB2	1.76	0.45
1:D:440:ARG:HD3	1:D:440:ARG:HA	1.59	0.45
1:A:346:GLU:HG2	1:B:345:MET:SD	2.58	0.44
1:F:493:LYS:HD3	3:F:601:PG4:H22	1.99	0.44
1:E:336:ALA:HA	1:E:339:GLU:OE2	2.18	0.44
1:E:338:LEU:HD12	1:E:338:LEU:HA	1.75	0.44
1:A:467:SER:OG	2:G:204:PRO:HB2	2.17	0.43
1:F:390:MET:HE3	1:F:390:MET:HB2	1.88	0.43
1:C:493:LYS:HZ2	4:C:602:PEG:H11	1.83	0.43
1:D:365:ARG:NH2	1:D:475:VAL:HG11	2.34	0.42
1:D:412:VAL:HG22	1:D:466:ALA:HB2	2.01	0.42
1:D:497:ASP:OD2	1:D:499:THR:OG1	2.20	0.42
1:D:345:MET:SD	1:F:346:GLU:HG3	2.60	0.42
1:A:382:TYR:HA	1:A:388:TYR:O	2.20	0.42
1:C:493:LYS:NZ	4:C:601:PEG:O2	2.52	0.42
1:F:396:LEU:HA	1:F:407:LEU:CD2	2.50	0.42
1:E:345:MET:HE2	1:E:345:MET:HB2	1.93	0.42
1:B:485:VAL:HG22	1:B:490:ILE:CG2	2.50	0.41
1:A:338:LEU:HD21	1:C:338:LEU:HD23	2.01	0.41
1:C:433:MET:HA	1:C:443:VAL:O	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:477:LYS:O	1:C:482:ASN:HB2	2.21	0.41
1:A:434:LEU:HB3	1:A:443:VAL:HB	2.03	0.41
1:C:382:TYR:HA	1:C:388:TYR:O	2.21	0.41
1:C:454:SER:HA	1:C:457:GLN:HG2	2.03	0.41
1:D:338:LEU:HD12	1:D:338:LEU:HA	1.76	0.41
1:F:375:ALA:HB2	1:F:395:TYR:CE1	2.55	0.41
1:F:433:MET:HA	1:F:443:VAL:O	2.21	0.41
1:A:412:VAL:HG22	1:A:466:ALA:HB2	2.03	0.41
1:B:433:MET:HA	1:B:443:VAL:O	2.20	0.41
1:B:454:SER:HA	1:B:457:GLN:HG2	2.02	0.41
1:D:479:GLU:HG3	1:D:480:ALA:H	1.86	0.41

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	166/188 (88%)	163 (98%)	3 (2%)	0	100	100
1	B	166/188 (88%)	164 (99%)	2 (1%)	0	100	100
1	C	166/188 (88%)	162 (98%)	4 (2%)	0	100	100
1	D	166/188 (88%)	165 (99%)	1 (1%)	0	100	100
1	E	166/188 (88%)	164 (99%)	2 (1%)	0	100	100
1	F	166/188 (88%)	163 (98%)	3 (2%)	0	100	100
2	G	3/5 (60%)	3 (100%)	0	0	100	100
2	H	3/5 (60%)	3 (100%)	0	0	100	100
2	I	3/5 (60%)	3 (100%)	0	0	100	100
All	All	1005/1143 (88%)	990 (98%)	15 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	144/162 (89%)	143 (99%)	1 (1%)	76	78
1	B	144/162 (89%)	143 (99%)	1 (1%)	76	78
1	C	144/162 (89%)	144 (100%)	0	100	100
1	D	144/162 (89%)	144 (100%)	0	100	100
1	E	144/162 (89%)	143 (99%)	1 (1%)	76	78
1	F	144/162 (89%)	142 (99%)	2 (1%)	59	59
2	G	4/4 (100%)	4 (100%)	0	100	100
2	H	4/4 (100%)	4 (100%)	0	100	100
2	I	4/4 (100%)	4 (100%)	0	100	100
All	All	876/984 (89%)	871 (99%)	5 (1%)	78	81

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	481	LYS
1	B	343	LEU
1	E	451	VAL
1	F	438	ASN
1	F	441	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	461	ASN
1	B	439	ASN
1	C	442	HIS
1	C	482	ASN
1	D	439	ASN
1	E	418	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

8 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	601	-	6,6,6	0.20	0	5,5,5	0.08	0
3	PG4	F	601	-	12,12,12	0.25	0	11,11,11	0.36	0
3	PG4	A	601	-	12,12,12	0.20	0	11,11,11	0.55	0
4	PEG	C	602	-	6,6,6	0.17	0	5,5,5	0.18	0
4	PEG	E	601	-	6,6,6	0.09	0	5,5,5	0.22	0
4	PEG	E	602	-	6,6,6	0.14	0	5,5,5	0.17	0
3	PG4	D	601	-	12,12,12	0.20	0	11,11,11	0.46	0
3	PG4	B	601	-	12,12,12	0.23	0	11,11,11	0.39	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	601	-	-	0/4/4/4	-
3	PG4	F	601	-	-	5/10/10/10	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PG4	A	601	-	-	1/10/10/10	-
4	PEG	C	602	-	-	2/4/4/4	-
4	PEG	E	601	-	-	2/4/4/4	-
4	PEG	E	602	-	-	2/4/4/4	-
3	PG4	D	601	-	-	3/10/10/10	-
3	PG4	B	601	-	-	8/10/10/10	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	F	601	PG4	O2-C3-C4-O3
3	B	601	PG4	O1-C1-C2-O2
4	C	602	PEG	O1-C1-C2-O2
4	E	601	PEG	O1-C1-C2-O2
3	B	601	PG4	C8-C7-O4-C6
3	B	601	PG4	O4-C7-C8-O5
3	D	601	PG4	O2-C3-C4-O3
4	E	601	PEG	O2-C3-C4-O4
3	B	601	PG4	C3-C4-O3-C5
3	F	601	PG4	C1-C2-O2-C3
4	E	602	PEG	O1-C1-C2-O2
3	B	601	PG4	C1-C2-O2-C3
3	F	601	PG4	C4-C3-O2-C2
3	B	601	PG4	C5-C6-O4-C7
3	D	601	PG4	O1-C1-C2-O2
4	C	602	PEG	C1-C2-O2-C3
3	D	601	PG4	C4-C3-O2-C2
3	B	601	PG4	C4-C3-O2-C2
3	F	601	PG4	C8-C7-O4-C6
3	F	601	PG4	C5-C6-O4-C7
4	E	602	PEG	C4-C3-O2-C2
3	B	601	PG4	O3-C5-C6-O4
3	A	601	PG4	O3-C5-C6-O4

There are no ring outliers.

5 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	601	PEG	1	0
3	F	601	PG4	1	0
3	A	601	PG4	1	0
4	C	602	PEG	2	0
3	B	601	PG4	3	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	168/188 (89%)	0.39	11 (6%)	25 26	26, 35, 63, 86	7 (4%)
1	B	168/188 (89%)	0.45	14 (8%)	17 18	25, 35, 67, 95	6 (3%)
1	C	168/188 (89%)	0.66	20 (11%)	9 9	26, 36, 80, 123	3 (1%)
1	D	168/188 (89%)	1.10	30 (17%)	3 3	32, 50, 95, 128	1 (0%)
1	E	168/188 (89%)	0.32	16 (9%)	14 14	24, 32, 70, 104	3 (1%)
1	F	168/188 (89%)	1.03	25 (14%)	5 6	28, 48, 74, 118	3 (1%)
2	G	5/5 (100%)	1.77	1 (20%)	3 2	30, 32, 42, 53	3 (60%)
2	H	5/5 (100%)	4.36	5 (100%)	0 0	43, 45, 66, 74	3 (60%)
2	I	5/5 (100%)	3.13	3 (60%)	0 0	50, 60, 71, 91	2 (40%)
All	All	1023/1143 (89%)	0.69	125 (12%)	8 9	24, 38, 80, 128	31 (3%)

All (125) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	439	ASN	8.3
1	F	334	ALA	6.3
2	H	207	ALA	6.2
2	H	205	ILE	5.9
1	E	334	ALA	5.6
1	B	334	ALA	5.0
2	I	205	ILE	4.9
1	C	334	ALA	4.9
1	F	335	MET	4.9
1	C	480	ALA	4.8
1	C	479	GLU	4.6
1	A	334	ALA	4.5
1	D	335	MET	4.5
1	D	343	LEU	4.4
1	F	423	ARG	4.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	I	207	ALA	4.3
1	D	344	GLU	4.3
1	E	335	MET	4.2
1	D	480	ALA	4.1
1	E	440	ARG	3.9
1	D	334	ALA	3.9
1	D	338	LEU	3.8
1	D	336	ALA	3.8
1	C	440	ARG	3.7
1	E	439	ASN	3.7
1	D	481	LYS	3.6
1	F	440	ARG	3.6
1	D	479	GLU	3.5
1	F	336	ALA	3.5
1	C	482	ASN	3.5
1	D	369	VAL	3.5
2	H	206	GLN	3.5
1	A	480	ALA	3.5
1	B	335	MET	3.5
1	C	478	MET	3.5
1	A	336	ALA	3.5
1	E	338	LEU	3.4
2	H	204	PRO	3.4
1	C	481	LYS	3.2
1	C	343	LEU	3.2
1	D	372	ARG	3.2
2	G	207	ALA	3.1
1	D	342	VAL	3.1
1	C	438	ASN	3.1
1	D	501	LEU	3.1
1	C	441	GLU	3.0
1	D	477	LYS	3.0
1	B	440	ARG	3.0
1	B	438	ASN	3.0
1	F	343	LEU	3.0
1	C	484	TYR	3.0
1	B	480	ALA	3.0
1	D	423	ARG	2.9
1	E	441	GLU	2.9
2	H	208	SER	2.9
1	F	438	ASN	2.8
1	F	407	LEU	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	439	ASN	2.8
1	D	370	ALA	2.8
1	F	370	ALA	2.8
1	E	340	GLN	2.8
1	D	476	SER	2.8
1	B	336	ALA	2.8
1	C	500	GLY	2.8
1	F	462	ASP	2.8
1	A	481	LYS	2.7
1	D	451	VAL	2.7
1	F	486	ARG	2.7
1	E	501	LEU	2.7
2	I	208	SER	2.6
1	A	335	MET	2.6
1	F	342	VAL	2.6
1	F	465	ILE	2.6
1	E	403	ARG	2.6
1	B	340	GLN	2.6
1	F	451	VAL	2.6
1	F	374	PRO	2.6
1	F	338	LEU	2.6
1	D	402	GLY	2.6
1	F	371	GLY	2.6
1	D	337	ASP	2.5
1	F	360	ASP	2.5
1	C	475	VAL	2.5
1	D	403	ARG	2.5
1	E	401	THR	2.4
1	D	371	GLY	2.4
1	E	438	ASN	2.4
1	C	335	MET	2.4
1	E	337	ASP	2.4
1	B	439	ASN	2.4
1	F	395	TYR	2.4
1	A	337	ASP	2.4
1	F	373	ILE	2.4
1	D	340	GLN	2.4
1	F	444	ILE	2.3
1	D	478	MET	2.3
1	D	465	ILE	2.3
1	B	481	LYS	2.3
1	A	501	LEU	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	482	ASN	2.3
1	C	483	SER	2.2
1	B	478	MET	2.2
1	B	501	LEU	2.2
1	E	343	LEU	2.2
1	C	476	SER	2.2
1	C	336	ALA	2.2
1	D	347	ALA	2.2
1	E	341	LYS	2.2
1	E	372	ARG	2.2
1	F	469	CYS	2.2
1	A	343	LEU	2.2
1	B	372	ARG	2.2
1	C	345	MET	2.2
1	C	445	ASP	2.2
1	F	454	SER	2.2
1	D	460	VAL	2.1
1	A	478	MET	2.1
1	A	407	LEU	2.1
1	B	403	ARG	2.1
1	D	440	ARG	2.1
1	F	372	ARG	2.1
1	B	482	ASN	2.1
1	E	336	ALA	2.1
1	A	440	ARG	2.0
1	D	405	THR	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
4	PEG	C	601	7/7	0.72	0.17	42,46,49,49	0
4	PEG	E	602	7/7	0.76	0.18	43,44,46,50	7
3	PG4	D	601	13/13	0.78	0.18	40,43,46,48	13
4	PEG	E	601	7/7	0.79	0.17	43,45,45,47	0
3	PG4	A	601	13/13	0.84	0.14	36,39,42,44	13
4	PEG	C	602	7/7	0.87	0.12	44,47,49,54	0
3	PG4	F	601	13/13	0.87	0.13	43,45,48,51	0
3	PG4	B	601	13/13	0.87	0.12	42,45,49,50	0

6.5 Other polymers [i](#)

There are no such residues in this entry.