



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:27 PM UTC

PDB ID : 3MC0 / pdb_00003mc0
Title : Crystal Structure of Staphylococcal Enterotoxin G (SEG) in Complex with a Mouse T-cell Receptor beta Chain
Authors : Fernandez, M.M.; Cho, S.; Robinson, H.; Mariuzza, R.A.; Malchiodi, E.L.
Deposited on : 2010-03-26
Resolution : 2.00 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

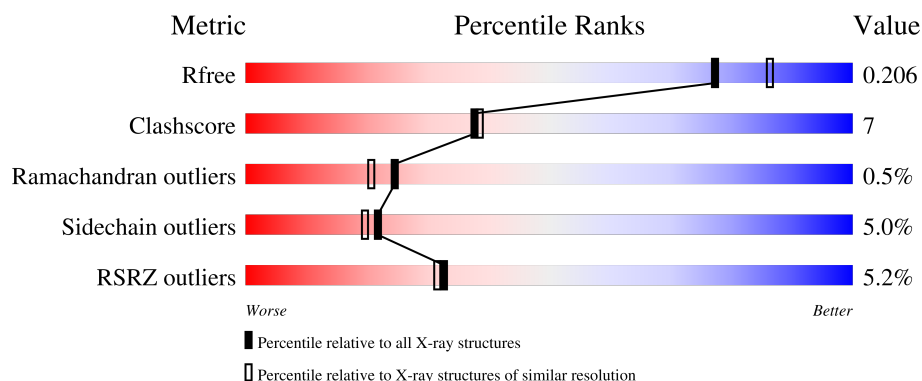
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	109	0% 83% 17% .
1	C	109	6% 83% 15% .
2	B	239	6% 68% 23% 5%
2	D	239	5% 75% 16% 5%

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
3	ACT	B	301	-	X	-	-
3	ACT	B	302	-	X	-	-
3	ACT	C	201	-	-	X	-
3	ACT	D	301	-	X	-	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5841 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 variable beta 8.2 mouse T cell receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	109	Total	C	N	O	S	0	0	0
			828	513	147	165	3			
1	C	109	Total	C	N	O	S	0	0	0
			828	513	147	165	3			

There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	17	GLU	GLY	engineered mutation	UNP A2NTY6
A	24	GLN	ASN	engineered mutation	UNP A2NTY6
A	73	GLN	ASN	engineered mutation	UNP A2NTY6
A	80	SER	LEU	engineered mutation	UNP A2NTY6
A	?	-	GLU	deletion	UNP A2NTY6
A	?	-	LEU	deletion	UNP A2NTY6
A	?	-	PHE	deletion	UNP A2NTY6
A	?	-	ASN	deletion	UNP A2NTY6
A	?	-	GLN	deletion	UNP A2NTY6
A	97	GLY	ASP	engineered mutation	UNP A2NTY6
A	99	LEU	GLN	engineered mutation	UNP A2NTY6
A	109	ALA	PRO	engineered mutation	UNP A2NTY6
A	114	SER	LEU	engineered mutation	UNP A2NTY6
C	17	GLU	GLY	engineered mutation	UNP A2NTY6
C	24	GLN	ASN	engineered mutation	UNP A2NTY6
C	73	GLN	ASN	engineered mutation	UNP A2NTY6
C	80	SER	LEU	engineered mutation	UNP A2NTY6
C	?	-	GLU	deletion	UNP A2NTY6
C	?	-	LEU	deletion	UNP A2NTY6
C	?	-	PHE	deletion	UNP A2NTY6
C	?	-	ASN	deletion	UNP A2NTY6
C	?	-	GLN	deletion	UNP A2NTY6
C	97	GLY	ASP	engineered mutation	UNP A2NTY6
C	99	LEU	GLN	engineered mutation	UNP A2NTY6
C	109	ALA	PRO	engineered mutation	UNP A2NTY6

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Chain	Residue	Modelled	Actual	Comment	Reference
C	114	SER	LEU	engineered mutation	UNP A2NTY6

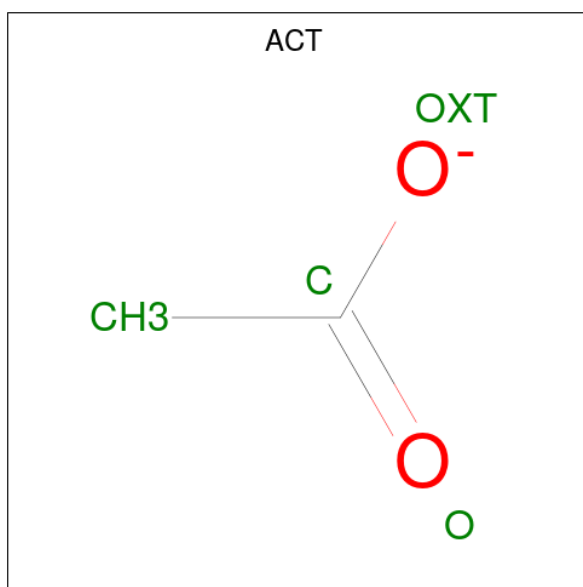
- Molecule 2 is a protein called Enterotoxin SEG.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	228	Total	C	N	O	S	0	0	0
			1862	1199	300	354	9			
2	D	227	Total	C	N	O	S	0	0	0
			1853	1194	298	352	9			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	234	HIS	-	expression tag	UNP D0EMB6
B	235	HIS	-	expression tag	UNP D0EMB6
B	236	HIS	-	expression tag	UNP D0EMB6
B	237	HIS	-	expression tag	UNP D0EMB6
B	238	HIS	-	expression tag	UNP D0EMB6
B	239	HIS	-	expression tag	UNP D0EMB6
D	234	HIS	-	expression tag	UNP D0EMB6
D	235	HIS	-	expression tag	UNP D0EMB6
D	236	HIS	-	expression tag	UNP D0EMB6
D	237	HIS	-	expression tag	UNP D0EMB6
D	238	HIS	-	expression tag	UNP D0EMB6
D	239	HIS	-	expression tag	UNP D0EMB6

- Molecule 3 is ACETATE ION (CCD ID: ACT) (formula: C₂H₃O₂).



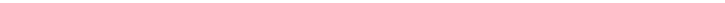
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	C	1	Total	C	O	0	0
			4	2	2		
3	D	1	Total	C	O	0	0
			4	2	2		
3	D	1	Total	C	O	0	0
			4	2	2		
3	D	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is water.

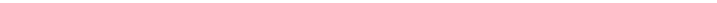
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	92	Total	O	0	0
			92	92		
4	B	121	Total	O	0	0
			121	121		
4	C	84	Total	O	0	0
			84	84		
4	D	141	Total	O	0	0
			141	141		

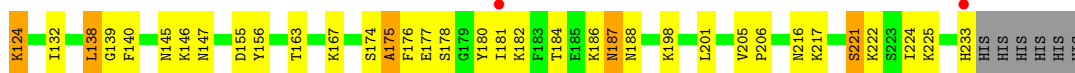
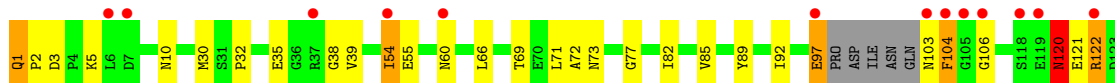
- Molecule 1: variable beta 8.2 mouse T cell receptor

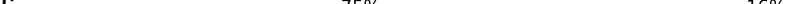


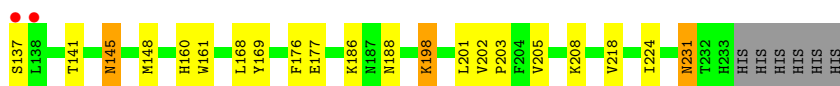
Chain C:  6% 83% 15%



Chain B:  6% 68% 23% 5%



Chain D:  5% 75% 16% 5%



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	91.19Å 91.19Å 233.40Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.90 – 2.00 29.90 – 2.00	Depositor EDS
% Data completeness (in resolution range)	93.9 (29.90-2.00) 93.9 (29.90-2.00)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	8.38 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.179 , 0.211 0.176 , 0.206	Depositor DCC
R_{free} test set	3634 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	34.1	Xtriage
Anisotropy	0.168	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 38.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.022 for -h,-k,l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	5841	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.48% 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: ACT

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	1.70	10/846 (1.2%)	1.36	1/1145 (0.1%)
1	C	1.71	7/846 (0.8%)	1.36	3/1145 (0.3%)
2	B	1.72	22/1906 (1.2%)	1.42	15/2570 (0.6%)
2	D	1.71	22/1897 (1.2%)	1.42	13/2557 (0.5%)
All	All	1.71	61/5495 (1.1%)	1.40	32/7417 (0.4%)

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
2	B	0	1

All (61) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	32	PRO	CA-C	11.63	1.58	1.51
1	A	100	TYR	C-N	8.25	1.44	1.33
2	D	224	ILE	CA-CB	7.88	1.62	1.54
1	C	100	TYR	C-N	7.87	1.44	1.33
2	D	168	LEU	N-CA	7.22	1.55	1.46
2	D	54	ILE	C-O	7.13	1.31	1.23
2	D	53	PRO	CA-C	-6.85	1.46	1.53
2	D	161	TRP	N-CA	6.61	1.54	1.46
1	A	27	ASN	CG-OD1	6.60	1.36	1.23
1	C	98	THR	CA-CB	6.54	1.63	1.53
2	B	177	GLU	CA-C	6.42	1.60	1.52
2	D	67	GLU	CA-C	6.40	1.61	1.52
2	D	231	ASN	N-CA	-6.38	1.38	1.46
2	B	54	ILE	CA-CB	6.33	1.61	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	178	SER	C-O	6.31	1.30	1.23
1	A	24	GLN	CB-CG	-6.27	1.33	1.52
2	B	104	PHE	CA-C	6.24	1.61	1.52
1	C	79	GLU	C-O	-6.11	1.16	1.24
2	B	224	ILE	CA-CB	6.08	1.60	1.54
2	B	180	TYR	CA-C	-5.99	1.45	1.52
2	B	140	PHE	CA-C	-5.91	1.45	1.52
2	D	128	VAL	CA-CB	5.85	1.61	1.54
1	C	88	VAL	CA-C	5.83	1.59	1.52
1	C	35	TYR	CA-C	5.81	1.60	1.52
1	A	26	THR	CA-CB	5.80	1.62	1.53
2	B	174	SER	CA-C	5.70	1.59	1.52
2	B	73	ASN	C-O	-5.69	1.17	1.24
2	B	139	GLY	CA-C	-5.69	1.46	1.52
1	A	14	VAL	CA-CB	5.67	1.62	1.54
2	D	24	ASN	N-CA	5.67	1.53	1.46
1	A	10	ASN	CA-C	-5.66	1.45	1.52
2	D	106	GLY	C-O	5.58	1.30	1.23
1	A	98	THR	CA-C	5.55	1.59	1.52
2	D	198	LYS	CA-C	-5.54	1.45	1.52
2	B	54	ILE	C-O	5.51	1.30	1.24
2	B	60	ASN	N-CA	5.50	1.53	1.46
2	B	181	ILE	CA-C	5.50	1.59	1.52
2	B	156	TYR	CA-C	5.48	1.59	1.52
1	A	75	SER	N-CA	5.46	1.52	1.46
2	D	160	HIS	CA-C	5.45	1.59	1.52
2	D	34	VAL	CA-CB	5.43	1.61	1.54
2	B	132	ILE	CA-CB	5.40	1.61	1.54
1	A	44	ARG	CB-CG	5.36	1.68	1.52
1	A	109	ALA	CA-CB	5.35	1.62	1.53
2	D	93	ILE	CG1-CD1	5.35	1.72	1.51
2	B	38	GLY	N-CA	5.35	1.53	1.45
1	C	17	GLU	CA-C	5.33	1.59	1.52
2	D	176	PHE	CA-C	-5.32	1.46	1.52
2	D	169	TYR	CA-C	5.30	1.59	1.52
2	B	106	GLY	C-O	5.27	1.31	1.24
2	B	175	ALA	N-CA	5.22	1.53	1.46
2	D	208	LYS	CD-CE	5.20	1.68	1.52
2	D	22	MET	CG-SD	5.19	1.93	1.80
2	D	61	GLU	CA-C	-5.18	1.46	1.52
1	C	35	TYR	CD2-CE2	5.13	1.54	1.38
2	B	32	PRO	CA-C	5.11	1.56	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	35	GLU	N-CA	5.10	1.52	1.46
2	D	177	GLU	CA-C	5.10	1.59	1.52
2	D	131	THR	CA-C	-5.08	1.46	1.52
2	B	198	LYS	CA-C	-5.07	1.46	1.52
2	B	69	THR	CA-CB	5.03	1.61	1.53

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	55	GLU	N-CA-C	11.68	127.12	109.25
2	D	53	PRO	CB-CA-C	-9.07	101.00	112.89
2	B	221	SER	CB-CA-C	-8.86	96.64	110.81
2	D	96	SER	N-CA-C	8.82	120.58	110.97
2	B	55	GLU	N-CA-C	8.15	122.52	110.30
2	D	188	ASN	N-CA-C	7.74	122.07	112.47
2	B	139	GLY	N-CA-C	-7.50	99.79	110.96
2	B	138	LEU	CA-C-N	-6.86	114.29	121.35
2	B	138	LEU	C-N-CA	-6.86	114.29	121.35
2	B	205	VAL	CA-C-N	6.81	126.61	119.05
2	B	205	VAL	C-N-CA	6.81	126.61	119.05
2	D	53	PRO	CA-C-O	-6.71	113.78	121.97
1	A	95	GLY	N-CA-C	-6.62	97.50	113.18
2	D	93	ILE	CB-CA-C	-6.52	99.50	111.36
2	B	104	PHE	N-CA-CB	-6.25	99.93	110.49
2	D	137	SER	N-CA-C	6.12	121.81	113.97
2	D	47	SER	CA-CB-OG	-5.92	99.27	111.10
2	B	176	PHE	N-CA-C	5.90	118.81	110.14
2	D	93	ILE	CG1-CB-CG2	-5.73	93.52	110.70
2	B	177	GLU	N-CA-C	-5.50	107.11	113.88
2	D	67	GLU	N-CA-C	-5.49	105.45	111.82
2	B	38	GLY	CA-C-N	-5.48	116.29	122.48
2	B	38	GLY	C-N-CA	-5.48	116.29	122.48
2	D	93	ILE	CB-CG1-CD1	-5.46	102.34	113.80
1	C	99	LEU	N-CA-C	5.43	118.39	109.76
1	C	22	SER	CB-CA-C	-5.37	99.54	109.37
1	C	35	TYR	CB-CA-C	-5.37	100.15	110.24
2	B	85	VAL	N-CA-CB	-5.36	105.25	111.20
2	D	82	ILE	CB-CA-C	-5.26	102.78	110.62
2	B	155	ASP	N-CA-C	-5.25	105.47	111.14
2	B	73	ASN	N-CA-C	-5.12	105.88	111.82
2	D	67	GLU	N-CA-CB	-5.07	102.42	110.28

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	103	ASN	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	828	0	788	5	0
1	C	828	0	788	7	0
2	B	1862	0	1829	36	0
2	D	1853	0	1819	20	0
3	A	8	0	6	2	0
3	B	8	0	6	1	0
3	C	4	0	3	3	0
3	D	12	0	9	1	0
4	A	92	0	0	2	0
4	B	121	0	0	5	0
4	C	84	0	0	4	0
4	D	141	0	0	5	0
All	All	5841	0	5248	74	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 7.

All (74) 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)
2:D:74:ASN:HB2	4:D:529:HOH:O	1.32	1.29
2:D:74:ASN:CB	4:D:529:HOH:O	1.99	0.95
2:D:127:THR:HG22	2:D:141:THR:HG22	1.49	0.95
2:B:120:ASN:HD21	2:B:147:ASN:H	1.11	0.92
3:A:201:ACT:H1	4:A:339:HOH:O	1.83	0.79
2:B:147:ASN:HD22	2:B:222:LYS:HE3	1.48	0.77
1:A:28:ASN:ND2	1:A:71:GLN:HG2	1.99	0.76
2:B:147:ASN:ND2	2:B:222:LYS:HE3	1.99	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:122:ARG:O	2:B:124:LYS:NZ	2.23	0.71
3:C:201:ACT:H1	4:C:354:HOH:O	1.90	0.71
1:A:2:ALA:N	4:A:377:HOH:O	2.24	0.71
2:B:120:ASN:ND2	2:B:147:ASN:H	1.87	0.71
2:B:124:LYS:HE3	2:B:147:ASN:ND2	2.05	0.70
2:B:1:GLN:HG2	2:B:1:GLN:O	1.91	0.70
2:B:77:GLY:O	4:B:520:HOH:O	2.12	0.68
2:B:146:LYS:O	2:B:221:SER:OG	2.10	0.67
3:A:202:ACT:H1	4:B:451:HOH:O	1.94	0.67
1:C:29:HIS:HD2	1:C:93:SER:OG	1.81	0.64
2:B:1:GLN:N	2:B:2:PRO:HA	2.14	0.62
1:C:94:GLY:HA3	4:C:344:HOH:O	2.00	0.61
2:B:92:ILE:HD12	2:B:104:PHE:HE2	1.67	0.59
1:A:28:ASN:HD22	1:A:71:GLN:HG2	1.66	0.59
2:D:55:GLU:O	2:D:55:GLU:HG3	2.02	0.58
2:D:145:ASN:OD1	2:D:145:ASN:C	2.46	0.58
2:D:54:ILE:O	2:D:54:ILE:HG12	2.06	0.55
2:B:2:PRO:HB2	4:B:420:HOH:O	2.07	0.54
2:B:66:LEU:HD13	2:B:72:ALA:HA	1.88	0.54
3:C:201:ACT:H2	4:D:453:HOH:O	2.07	0.53
2:B:124:LYS:HE3	2:B:147:ASN:HD21	1.74	0.52
2:B:124:LYS:HG3	2:B:221:SER:HB2	1.91	0.52
2:B:233:HIS:CD2	2:B:233:HIS:C	2.87	0.52
2:B:1:GLN:O	2:B:1:GLN:CG	2.57	0.51
2:B:184:THR:HB	2:B:225:LYS:HB3	1.93	0.50
2:D:53:PRO:C	2:D:54:ILE:CG2	2.85	0.49
2:D:54:ILE:O	2:D:54:ILE:CG1	2.58	0.49
2:B:39:VAL:HG21	2:B:82:ILE:CD1	2.43	0.49
2:B:30:MET:HG2	2:B:163:THR:HG21	1.95	0.49
2:D:38:GLY:HA2	2:D:79:LYS:HG2	1.94	0.49
2:D:74:ASN:ND2	4:D:529:HOH:O	2.46	0.49
2:D:74:ASN:CG	4:D:529:HOH:O	2.42	0.48
1:A:78:LEU:HD12	1:A:78:LEU:N	2.29	0.48
2:B:186:LYS:C	2:B:188:ASN:H	2.23	0.47
2:B:3:ASP:OD1	2:B:182:LYS:NZ	2.39	0.47
1:C:29:HIS:HB3	1:C:94:GLY:O	2.14	0.47
2:B:66:LEU:HD22	2:B:71:LEU:HG	1.97	0.46
1:C:50:TYR:OH	4:C:365:HOH:O	2.20	0.46
2:D:201:LEU:HD11	2:D:205:VAL:HB	1.96	0.46
1:A:24:GLN:HE21	1:A:24:GLN:HB2	1.50	0.46
1:C:28:ASN:HD22	1:C:71:GLN:HG2	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:145:ASN:OD1	2:B:145:ASN:C	2.57	0.46
2:B:217:LYS:NZ	4:B:505:HOH:O	2.50	0.45
2:D:95:LYS:HD3	2:D:95:LYS:HA	1.68	0.45
2:D:202:VAL:HA	2:D:203:PRO:C	2.42	0.45
2:B:124:LYS:HG3	2:B:221:SER:CB	2.47	0.44
2:B:1:GLN:H3	2:B:2:PRO:HA	1.82	0.44
2:B:10:ASN:ND2	4:B:445:HOH:O	2.49	0.43
2:B:92:ILE:HD12	2:B:104:PHE:CE2	2.49	0.43
2:B:187:ASN:O	2:B:188:ASN:CB	2.66	0.43
2:D:122:ARG:HA	2:D:122:ARG:HD3	1.73	0.42
2:D:53:PRO:C	2:D:54:ILE:HG23	2.43	0.42
2:B:97:GLU:H	2:B:97:GLU:CD	2.27	0.42
2:B:167:LYS:HB2	2:B:175:ALA:HB2	2.01	0.42
2:D:31:SER:HB3	2:D:32:PRO:HD2	2.02	0.42
2:B:201:LEU:HD12	2:B:201:LEU:HA	1.82	0.42
2:D:148:MET:HB3	2:D:218:VAL:CG1	2.49	0.42
2:D:127:THR:HG22	2:D:141:THR:CG2	2.35	0.42
3:B:302:ACT:H2	3:D:302:ACT:H1	2.01	0.42
2:B:30:MET:HE3	2:B:30:MET:HB3	1.91	0.41
3:C:201:ACT:O	4:C:380:HOH:O	2.22	0.41
2:B:186:LYS:O	2:B:188:ASN:N	2.54	0.41
1:C:27:ASN:OD1	1:C:27:ASN:N	2.53	0.41
2:B:89:TYR:O	2:B:206:PRO:HG2	2.21	0.40
1:C:31:ASN:HA	1:C:49:SER:O	2.22	0.40
2:D:93:ILE:HD12	2:D:93:ILE:HG21	1.54	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	107/109 (98%)	102 (95%)	4 (4%)	1 (1%)	14 9

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	107/109 (98%)	105 (98%)	2 (2%)	0	100	100
2	B	224/239 (94%)	212 (95%)	10 (4%)	2 (1%)	14	9
2	D	223/239 (93%)	213 (96%)	10 (4%)	0	100	100
All	All	661/696 (95%)	632 (96%)	26 (4%)	3 (0%)	24	21

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	187	ASN
1	A	96	GLY
2	B	120	ASN

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	88/88 (100%)	84 (96%)	4 (4%)	24	23
1	C	88/88 (100%)	83 (94%)	5 (6%)	18	15
2	B	211/222 (95%)	201 (95%)	10 (5%)	23	22
2	D	210/222 (95%)	199 (95%)	11 (5%)	21	18
All	All	597/620 (96%)	567 (95%)	30 (5%)	22	20

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	GLN
1	A	72	GLU
1	A	99	LEU
1	A	116	LEU
2	B	1	GLN
2	B	5	LYS
2	B	54	ILE
2	B	97	GLU

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Mol	Chain	Res	Type
2	B	120	ASN
2	B	121	GLU
2	B	122	ARG
2	B	124	LYS
2	B	138	LEU
2	B	216	ASN
1	C	24	GLN
1	C	27	ASN
1	C	72	GLU
1	C	98	THR
1	C	99	LEU
2	D	6	LEU
2	D	8	GLU
2	D	54	ILE
2	D	93	ILE
2	D	122	ARG
2	D	125	LEU
2	D	136	GLN
2	D	145	ASN
2	D	186	LYS
2	D	198	LYS
2	D	231	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	24	GLN
1	A	28	ASN
1	A	73	GLN
2	B	10	ASN
2	B	74	ASN
2	B	103	ASN
2	B	120	ASN
2	B	147	ASN
2	B	231	ASN
2	B	233	HIS
1	C	28	ASN
1	C	29	HIS
2	D	10	ASN
2	D	74	ASN
2	D	116	ASN
2	D	231	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$
3	ACT	D	301	-	3,3,3	2.59	3 (100%)	3,3,3	3.23	3 (100%)
3	ACT	B	301	-	3,3,3	3.02	1 (33%)	3,3,3	2.79	2 (66%)
3	ACT	D	302	-	3,3,3	1.83	1 (33%)	3,3,3	0.56	0
3	ACT	D	303	-	3,3,3	1.02	0	3,3,3	0.92	0
3	ACT	A	201	-	3,3,3	1.40	1 (33%)	3,3,3	1.43	0
3	ACT	C	201	-	3,3,3	1.27	0	3,3,3	3.86	2 (66%)
3	ACT	A	202	-	3,3,3	0.97	0	3,3,3	2.47	2 (66%)
3	ACT	B	302	-	3,3,3	2.57	2 (66%)	3,3,3	3.13	2 (66%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	301	ACT	O-C	5.20	1.44	1.22
3	D	302	ACT	O-C	3.04	1.35	1.22
3	D	301	ACT	CH3-C	2.99	1.60	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	302	ACT	O-C	2.94	1.35	1.22
3	B	302	ACT	OXT-C	2.89	1.44	1.30
3	D	301	ACT	O-C	2.47	1.33	1.22
3	D	301	ACT	OXT-C	2.26	1.41	1.30
3	A	201	ACT	O-C	2.23	1.32	1.22

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	201	ACT	OXT-C-O	-5.61	101.21	122.03
3	D	301	ACT	OXT-C-CH3	4.40	133.50	115.05
3	B	302	ACT	OXT-C-CH3	4.11	132.29	115.05
3	B	301	ACT	OXT-C-CH3	-3.61	99.91	115.05
3	B	302	ACT	O-C-CH3	-3.44	108.42	122.53
3	A	202	ACT	OXT-C-CH3	3.38	129.20	115.05
3	B	301	ACT	O-C-CH3	3.13	135.36	122.53
3	C	201	ACT	OXT-C-CH3	3.13	128.18	115.05
3	D	301	ACT	OXT-C-O	-2.61	112.34	122.03
3	D	301	ACT	O-C-CH3	-2.28	113.19	122.53
3	A	202	ACT	OXT-C-O	-2.18	113.94	122.03

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	302	ACT	1	0
3	A	201	ACT	1	0
3	C	201	ACT	3	0
3	A	202	ACT	1	0
3	B	302	ACT	1	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	109/109 (100%)	-0.44	1 (0%) 81 80	21, 30, 45, 55	0
1	C	109/109 (100%)	-0.18	6 (5%) 30 29	22, 32, 53, 67	0
2	B	228/239 (95%)	0.11	15 (6%) 24 23	20, 36, 69, 89	3 (1%)
2	D	227/239 (94%)	-0.04	13 (5%) 29 28	21, 32, 70, 83	2 (0%)
All	All	673/696 (96%)	-0.08	35 (5%) 33 31	20, 33, 64, 89	5 (0%)

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	6	LEU	7.5
2	D	2	PRO	5.1
2	B	97	GLU	4.3
2	B	54	ILE	4.2
2	B	104	PHE	3.9
2	B	37	ARG	3.8
2	D	122	ARG	3.8
1	C	95	GLY	3.7
2	B	103	ASN	3.6
1	C	2	ALA	3.6
1	C	96	GLY	3.6
2	D	97	GLU	3.2
1	A	96	GLY	3.2
2	B	60	ASN	3.1
2	D	137	SER	2.9
1	C	97	GLY	2.9
2	D	104	PHE	2.9
2	D	103	ASN	2.9
2	B	118	SER	2.8
1	C	98	THR	2.8
2	B	6	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
2	B	119	GLU	2.7
2	B	233	HIS	2.7
2	B	106	GLY	2.6
2	D	60	ASN	2.5
2	D	138	LEU	2.5
2	D	54	ILE	2.5
2	D	96	SER	2.4
2	B	105	GLY	2.4
2	D	105	GLY	2.3
2	B	181	ILE	2.3
2	D	106	GLY	2.3
2	B	7	ASP	2.2
1	C	26	THR	2.2
2	B	122	ARG	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	ACT	D	301	4/4	0.55	0.21	30,33,36,40	0
3	ACT	B	302	4/4	0.61	0.21	30,34,34,36	0
3	ACT	C	201	4/4	0.63	0.22	46,50,51,52	0
3	ACT	A	202	4/4	0.66	0.24	42,48,48,49	0
3	ACT	D	303	4/4	0.73	0.24	58,59,59,60	0
3	ACT	B	301	4/4	0.75	0.21	37,40,42,46	0
3	ACT	D	302	4/4	0.79	0.20	38,44,46,46	0
3	ACT	A	201	4/4	0.84	0.16	46,48,50,50	0

6.5 Other polymers [i](#)

There are no such residues in this entry.