



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 01:44 PM GMT

PDB ID : 3MC0
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 validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

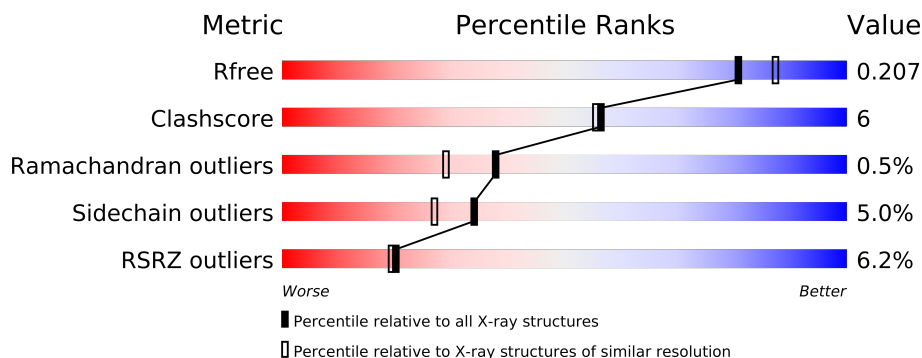
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

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}	66092	4888 (2.00-2.00)
Clashscore	79885	6188 (2.00-2.00)
Ramachandran outliers	78287	6102 (2.00-2.00)
Sidechain outliers	78261	6100 (2.00-2.00)
RSRZ outliers	66119	4890 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	109	
1	C	109	
2	B	239	
2	D	239	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
3	ACT	A	201	-	X
3	ACT	A	202	-	X
3	ACT	B	301	-	X
3	ACT	B	302	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
3	ACT	C	201	-	X
3	ACT	D	301	-	X
3	ACT	D	302	-	X
3	ACT	D	303	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5841 atoms, of which 0 are hydrogen and 0 are deuterium.

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

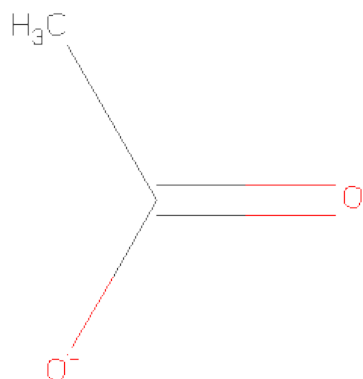
- Molecule 2 is a protein called Enterotoxin SEG.

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 (three-letter code: 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		

3 Residue-property plots

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

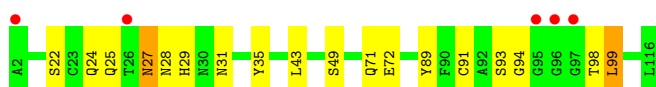
- Molecule 1: variable beta 8.2 mouse T cell receptor

Chain A: 



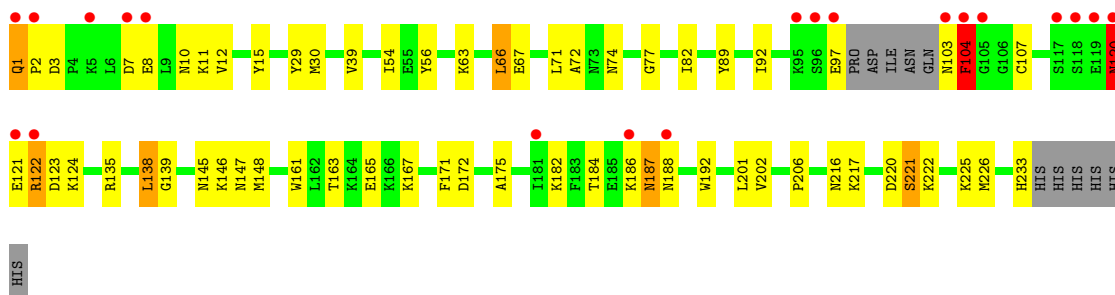
- Molecule 1: variable beta 8.2 mouse T cell receptor

Chain C: 



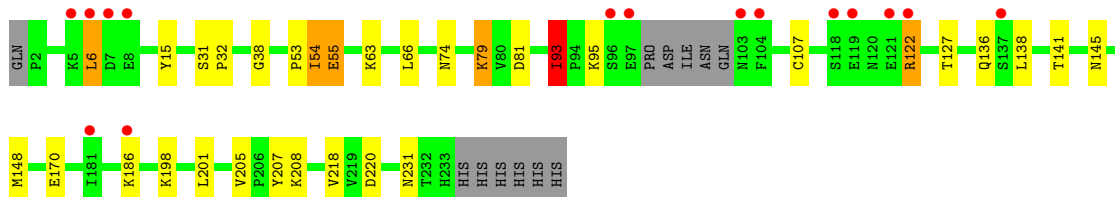
- Molecule 2: Enterotoxin SEG

Chain B: 



- Molecule 2: Enterotoxin SEG

Chain D: 



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 29.85 – 2.00	Depositor EDS
% Data completeness (in resolution range)	93.9 (29.90-2.00) 94.0 (29.85-2.00)	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 5.5.0109	Depositor
R, R_{free}	0.179 , 0.211 0.177 , 0.207	Depositor DCC
R_{free} test set	3634 reflections (5.32%)	DCC
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 , 41.9	EDS
Estimated twinning fraction	0.022 for -h,-k,l	Xtriage
L-test for twinning	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	1 of 71977 reflections (0.001%)	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.

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	1.51	9/846 (1.1%)	1.14	3/1145 (0.3%)
1	C	1.47	3/846 (0.4%)	1.18	6/1145 (0.5%)
2	B	1.50	18/1906 (0.9%)	1.15	12/2570 (0.5%)
2	D	1.45	6/1897 (0.3%)	1.17	9/2557 (0.4%)
All	All	1.48	36/5495 (0.7%)	1.16	30/7417 (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 (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	35	TYR	CD2-CE2	9.79	1.54	1.39
1	A	33	TYR	CD2-CE2	8.03	1.51	1.39
2	B	56	TYR	CD2-CE2	7.44	1.50	1.39
2	B	29	TYR	CD1-CE1	7.06	1.50	1.39
1	A	24	GLN	CB-CG	-7.01	1.33	1.52
2	B	15	TYR	CE2-CZ	6.97	1.47	1.38
2	D	107	CYS	CB-SG	-6.96	1.70	1.82
2	B	107	CYS	CB-SG	-6.84	1.70	1.82
2	D	208	LYS	CD-CE	6.72	1.68	1.51
2	D	207	TYR	CD1-CE1	6.70	1.49	1.39
1	C	91	CYS	CB-SG	-6.47	1.71	1.82
1	C	89	TYR	CE2-CZ	6.22	1.46	1.38
2	B	67	GLU	CG-CD	6.16	1.61	1.51
1	A	35	TYR	CD1-CE1	6.15	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	8	GLU	CG-CD	5.98	1.60	1.51
2	B	15	TYR	CD2-CE2	5.97	1.48	1.39
1	A	44	ARG	CB-CG	5.92	1.68	1.52
1	A	89	TYR	CE2-CZ	5.80	1.46	1.38
2	B	171	PHE	CE2-CZ	5.78	1.48	1.37
2	D	15	TYR	CE2-CZ	5.62	1.45	1.38
2	B	202	VAL	CB-CG1	5.61	1.64	1.52
2	B	221	SER	CB-OG	-5.61	1.34	1.42
2	B	165	GLU	CG-CD	5.55	1.60	1.51
1	A	27	ASN	CG-OD1	5.52	1.36	1.24
2	B	192	TRP	CB-CG	-5.46	1.40	1.50
2	D	170	GLU	CD-OE2	-5.46	1.19	1.25
2	B	11	LYS	CE-NZ	5.42	1.62	1.49
1	A	56	GLU	CB-CG	5.34	1.62	1.52
2	B	63	LYS	CD-CE	5.33	1.64	1.51
2	B	29	TYR	CD2-CE2	5.30	1.47	1.39
2	B	29	TYR	CE2-CZ	5.21	1.45	1.38
2	B	12	VAL	CB-CG1	5.20	1.63	1.52
2	B	161	TRP	CZ3-CH2	5.20	1.48	1.40
1	A	89	TYR	CG-CD1	5.10	1.45	1.39
1	A	35	TYR	CE2-CZ	5.09	1.45	1.38
2	D	63	LYS	CD-CE	5.08	1.64	1.51

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	93	ILE	CG1-CB-CG2	-8.13	93.52	111.40
2	D	138	LEU	CA-CB-CG	7.23	131.93	115.30
2	B	66	LEU	CB-CG-CD1	7.17	123.19	111.00
2	B	221	SER	CB-CA-C	-7.09	96.64	110.10
2	B	138	LEU	CA-CB-CG	6.97	131.33	115.30
2	D	66	LEU	CB-CG-CD1	6.60	122.23	111.00
2	D	66	LEU	CA-CB-CG	-6.52	100.31	115.30
1	A	43	LEU	CB-CG-CD1	-6.50	99.96	111.00
2	B	135	ARG	NE-CZ-NH1	6.46	123.53	120.30
1	C	43	LEU	CB-CG-CD1	6.31	121.72	111.00
1	A	95	GLY	N-CA-C	-6.24	97.50	113.10
1	C	43	LEU	CB-CG-CD2	6.08	121.33	111.00
2	B	123	ASP	CB-CG-OD2	6.06	123.76	118.30
2	D	93	ILE	CB-CA-C	-6.05	99.50	111.60
2	D	55	GLU	N-CA-C	5.97	127.12	111.00
2	B	104	PHE	N-CA-CB	-5.93	99.93	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	66	LEU	CA-CB-CG	-5.88	101.79	115.30
2	D	220	ASP	CB-CG-OD1	5.82	123.53	118.30
1	C	43	LEU	CA-CB-CG	5.66	128.32	115.30
2	B	220	ASP	CB-CG-OD2	-5.58	113.28	118.30
1	C	22	SER	CB-CA-C	-5.56	99.54	110.10
2	B	226	MET	CG-SD-CE	-5.54	91.34	100.20
2	B	172	ASP	CB-CG-OD1	5.39	123.15	118.30
2	D	81	ASP	CB-CG-OD2	-5.35	113.49	118.30
2	B	139	GLY	N-CA-C	-5.33	99.79	113.10
2	D	6	LEU	CB-CG-CD1	5.24	119.91	111.00
1	C	99	LEU	CB-CG-CD1	5.23	119.90	111.00
2	B	148	MET	CG-SD-CE	5.14	108.42	100.20
1	C	35	TYR	CB-CA-C	-5.12	100.15	110.40
1	A	77	ILE	CG1-CB-CG2	-5.05	100.30	111.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	103	ASN	Peptide

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	828	0	788	5	0
1	C	828	0	788	6	0
2	B	1862	0	1829	34	0
2	D	1853	0	1819	18	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	84	0	0	3	0
4	D	141	0	0	5	0
All	All	5841	0	5248	69	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 6.

All (69) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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
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:54:ILE:HG12	2:D:54:ILE:O	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:D:145:ASN:C	2:D:145:ASN:OD1	2.46	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:1:GLN:CG	2:B:1:GLN:O	2.57	0.51
2:B:184:THR:HB	2:B:225:LYS:HB3	1.93	0.50
2:D:54:ILE:CG1	2:D:54:ILE:O	2.58	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
1:A:78:LEU:N	1:A:78:LEU:HD12	2.29	0.48
2:B:233:HIS:C	2:B:233:HIS:CD2	2.87	0.47
1:C:29:HIS:HB3	1:C:94:GLY:O	2.14	0.47
2:B:3:ASP:OD1	2:B:182:LYS:NZ	2.39	0.47
2:B:66:LEU:HD22	2:B:71:LEU:HG	1.97	0.46
2:D:201:LEU:HD11	2:D:205:VAL:HB	1.96	0.46
1:A:24:GLN:HB2	1:A:24:GLN:HE21	1.50	0.46
1:C:28:ASN:HD22	1:C:71:GLN:HG2	1.81	0.46
2:D:95:LYS:HA	2:D:95:LYS:HD3	1.68	0.45
2:B:217:LYS:NZ	4:B:505:HOH:O	2.50	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:D:74:ASN:CG	4:D:529:HOH:O	2.42	0.43
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:B:186:LYS:C	2:B:188:ASN:H	2.23	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:CG2	2.85	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:D:148:MET:HB3	2:D:218:VAL:CG1	2.49	0.42
2:B:201:LEU:HA	2:B:201:LEU:HD12	1.82	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:145:ASN:C	2:B:145:ASN:OD1	2.57	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

5.3.1 Protein backbone ⓘ

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%)	25	14
1	C	107/109 (98%)	105 (98%)	2 (2%)	0	100	100
2	B	224/239 (94%)	212 (95%)	10 (4%)	2 (1%)	25	14
2	D	223/239 (93%)	213 (96%)	10 (4%)	0	100	100
All	All	661/696 (95%)	632 (96%)	26 (4%)	3 (0%)	38	29

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%)	38	31
1	C	88/88 (100%)	82 (93%)	6 (7%)	22	15
2	B	211/222 (95%)	200 (95%)	11 (5%)	32	25
2	D	210/222 (95%)	201 (96%)	9 (4%)	40	33
All	All	597/620 (96%)	567 (95%)	30 (5%)	34	27

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	7	ASP
2	B	54	ILE
2	B	74	ASN
2	B	97	GLU
2	B	104	PHE
2	B	120	ASN
2	B	121	GLU
2	B	122	ARG
2	B	138	LEU
2	B	216	ASN
1	C	24	GLN
1	C	25	GLN
1	C	27	ASN
1	C	72	GLU
1	C	98	THR
1	C	99	LEU
2	D	6	LEU
2	D	54	ILE
2	D	79	LYS
2	D	93	ILE
2	D	122	ARG
2	D	136	GLN
2	D	186	LYS
2	D	198	LYS
2	D	231	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) 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	120	ASN
2	B	147	ASN
2	B	233	HIS
1	C	28	ASN
1	C	29	HIS

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Mol	Chain	Res	Type
2	D	10	ASN
2	D	231	ASN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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	A	201	-	1,3,3	0.90	0	0,3,3	0.00	-
3	ACT	A	202	-	1,3,3	3.77	1 (100%)	0,3,3	0.00	-
3	ACT	B	301	-	1,3,3	1.61	0	0,3,3	0.00	-
3	ACT	B	302	-	1,3,3	4.85	1 (100%)	0,3,3	0.00	-
3	ACT	C	201	-	1,3,3	3.92	1 (100%)	0,3,3	0.00	-
3	ACT	D	301	-	1,3,3	8.52	1 (100%)	0,3,3	0.00	-
3	ACT	D	302	-	1,3,3	1.52	0	0,3,3	0.00	-
3	ACT	D	303	-	1,3,3	1.56	0	0,3,3	0.00	-

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical

component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ACT	A	201	-	-	0/0/0/0	0/0/0/0
3	ACT	A	202	-	-	0/0/0/0	0/0/0/0
3	ACT	B	301	-	-	0/0/0/0	0/0/0/0
3	ACT	B	302	-	-	0/0/0/0	0/0/0/0
3	ACT	C	201	-	-	0/0/0/0	0/0/0/0
3	ACT	D	301	-	-	0/0/0/0	0/0/0/0
3	ACT	D	302	-	-	0/0/0/0	0/0/0/0
3	ACT	D	303	-	-	0/0/0/0	0/0/0/0

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	301	ACT	CH3-C	8.52	1.60	1.48
3	B	302	ACT	CH3-C	4.85	1.55	1.48
3	C	201	ACT	CH3-C	3.92	1.54	1.48
3	A	202	ACT	CH3-C	3.77	1.54	1.48

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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%)	-0.43	2 (1%) 65 66	21, 30, 45, 55	0
1	C	109/109 (100%)	-0.32	5 (4%) 31 30	22, 32, 53, 67	0
2	B	228/239 (95%)	-0.04	20 (8%) 10 9	20, 36, 69, 89	3 (1%)
2	D	227/239 (94%)	-0.12	15 (6%) 18 17	22, 32, 70, 83	2 (0%)
All	All	673/696 (96%)	-0.18	42 (6%) 20 19	20, 33, 65, 89	5 (0%)

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	103	ASN	7.6
2	D	103	ASN	7.3
2	B	97	GLU	6.7
1	C	96	GLY	5.4
2	B	118	SER	5.1
2	B	119	GLU	4.9
2	B	122	ARG	4.6
1	C	95	GLY	4.6
2	B	104	PHE	4.0
2	D	7	ASP	4.0
2	D	97	GLU	3.8
2	D	122	ARG	3.5
2	B	96	SER	3.4
2	D	5	LYS	3.3
1	C	2	ALA	3.2
2	D	119	GLU	3.1
2	D	121	GLU	3.0
1	C	26	THR	3.0
2	D	104	PHE	2.9
2	D	6	LEU	2.8
2	D	181	ILE	2.7

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Mol	Chain	Res	Type	RSRZ
2	B	121	GLU	2.7
2	B	188	ASN	2.6
2	B	2	PRO	2.5
2	B	117	SER	2.5
2	D	118	SER	2.5
2	B	186	LYS	2.5
2	D	186	LYS	2.5
2	D	96	SER	2.4
2	B	7	ASP	2.4
2	B	120	ASN	2.4
2	B	5	LYS	2.3
2	B	105	GLY	2.3
2	B	1	GLN	2.3
1	A	2	ALA	2.2
2	B	181	ILE	2.2
2	D	8	GLU	2.2
2	B	95	LYS	2.2
2	D	137	SER	2.2
1	A	96	GLY	2.1
2	B	8	GLU	2.1
1	C	97	GLY	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	ACT	D	302	4/4	0.20	12.73	38,44,46,46	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	ACT	B	302	4/4	0.21	11.41	30,34,34,36	0
3	ACT	D	303	4/4	0.18	9.73	58,59,59,60	0
3	ACT	A	202	4/4	0.23	8.24	42,48,48,49	0
3	ACT	C	201	4/4	0.21	7.50	46,50,51,52	0
3	ACT	D	301	4/4	0.20	6.87	30,33,36,40	0
3	ACT	B	301	4/4	0.20	5.69	37,40,42,46	0
3	ACT	A	201	4/4	0.12	2.11	46,48,50,50	0

6.5 Other polymers ⓘ

There are no such residues in this entry.