



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 05:47 AM UTC

PDB ID : 4ODB / pdb_00004odb
Title : Crystal structure of the T1L reovirus attachment protein sigma1 in complex with Junctional Adhesion Molecule-A
Authors : Stettner, E.; Stehle, T.
Deposited on : 2014-01-10
Resolution : 3.20 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:

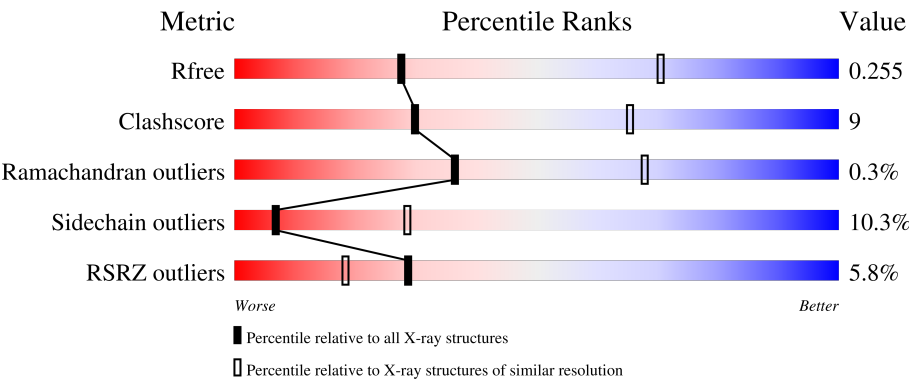
MolProbity : 4-5-2 with Phenix2.0
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)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

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

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	165	71%21%5%..
1	B	165	70%22%..
1	C	165	71%22%..
2	D	104	75%20%..
2	E	104	74%22%..

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Mol	Chain	Length	Quality of chain
2	F	104	19% 75% 21% • •

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6276 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 Outer capsid protein sigma-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	162	Total	C	N	O	S	0	0	0
			1294	824	217	246	7			
1	B	162	Total	C	N	O	S	0	0	0
			1294	824	217	246	7			
1	C	162	Total	C	N	O	S	0	0	0
			1294	824	217	246	7			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	306	MET	-	expression tag	UNP P04506
A	307	GLU	-	expression tag	UNP P04506
B	306	MET	-	expression tag	UNP P04506
B	307	GLU	-	expression tag	UNP P04506
C	306	MET	-	expression tag	UNP P04506
C	307	GLU	-	expression tag	UNP P04506

- Molecule 2 is a protein called Junctional adhesion molecule A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	102	Total	C	N	O	S	0	0	0
			798	500	132	162	4			
2	E	102	Total	C	N	O	S	0	0	0
			798	500	132	162	4			
2	F	102	Total	C	N	O	S	0	0	0
			798	500	132	162	4			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	26	GLY	-	expression tag	UNP Q9Y624
D	27	SER	-	expression tag	UNP Q9Y624

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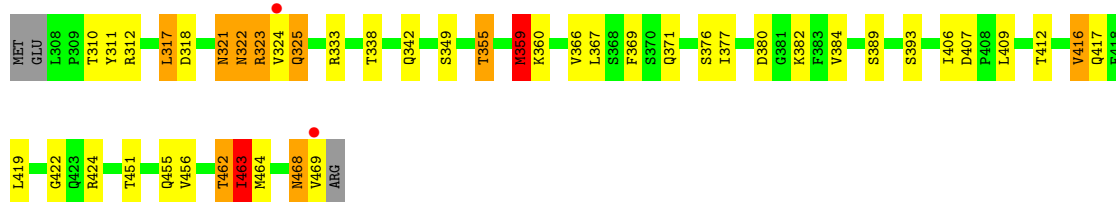
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Chain	Residue	Modelled	Actual	Comment	Reference
E	26	GLY	-	expression tag	UNP Q9Y624
E	27	SER	-	expression tag	UNP Q9Y624
F	26	GLY	-	expression tag	UNP Q9Y624
F	27	SER	-	expression tag	UNP Q9Y624

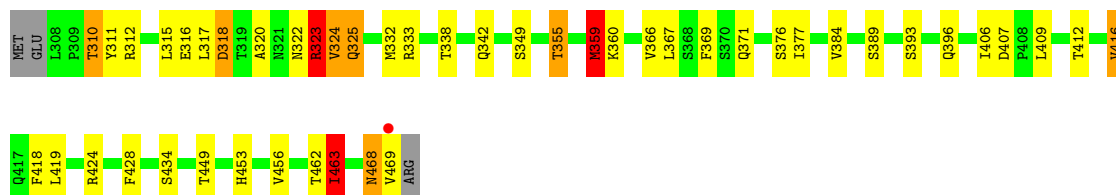
3 Residue-property plots [i](#)

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.

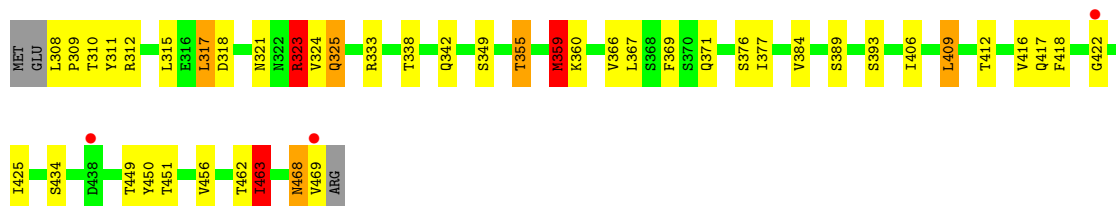
- Molecule 1: Outer capsid protein sigma-1



- Molecule 1: Outer capsid protein sigma-1

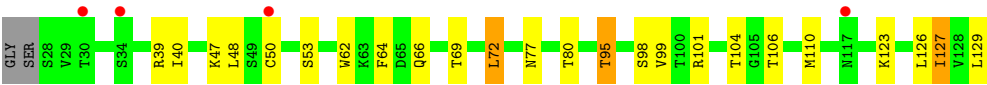


- Molecule 1: Outer capsid protein sigma-1



- Molecule 2: Junctional adhesion molecule A

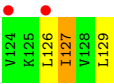
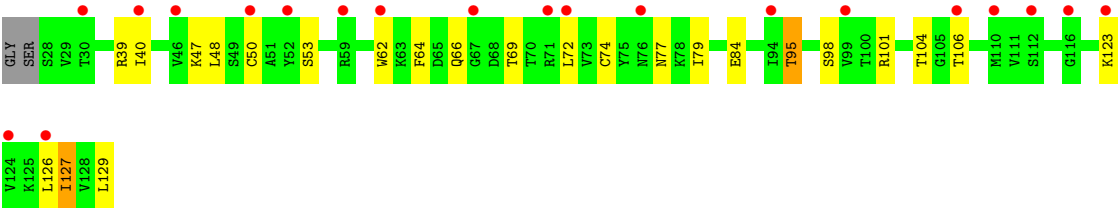
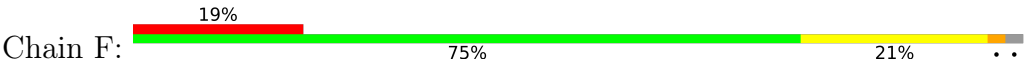




● Molecule 2: Junctional adhesion molecule A



● Molecule 2: Junctional adhesion molecule A



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	156.77Å 156.77Å 96.54Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	40.98 – 3.20 40.98 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.2 (40.98-3.20) 99.1 (40.98-3.20)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.47 (at 3.18Å)	Xtriage
Refinement program	BUSTER 2.10.0	Depositor
R, R_{free}	0.211 , 0.242 0.221 , 0.255	Depositor DCC
R_{free} test set	2268 reflections (10.00%)	wwPDB-VP
Wilson B-factor (Å ²)	68.6	Xtriage
Anisotropy	0.707	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 75.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.026 for -h,-k,l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	6276	wwPDB-VP
Average B, all atoms (Å ²)	81.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.04% 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

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	0.87	3/1330 (0.2%)	1.28	17/1817 (0.9%)
1	B	0.83	1/1330 (0.1%)	1.25	12/1817 (0.7%)
1	C	0.80	1/1330 (0.1%)	1.27	9/1817 (0.5%)
2	D	0.77	1/814 (0.1%)	1.19	2/1104 (0.2%)
2	E	0.70	0/814	1.19	2/1104 (0.2%)
2	F	0.70	0/814	1.20	2/1104 (0.2%)
All	All	0.79	6/6432 (0.1%)	1.24	44/8763 (0.5%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	359	MET	SD-CE	-7.73	1.60	1.79
1	A	468	ASN	CA-C	6.27	1.60	1.52
1	A	359	MET	SD-CE	-6.09	1.64	1.79
1	B	359	MET	SD-CE	-5.42	1.66	1.79
2	D	110	MET	SD-CE	5.40	1.93	1.79
1	A	464	MET	SD-CE	-5.09	1.66	1.79

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	310	THR	N-CA-C	-7.63	100.69	110.53
1	A	468	ASN	CA-C-N	7.61	135.40	121.70
1	A	468	ASN	C-N-CA	7.61	135.40	121.70
1	B	468	ASN	CA-C-N	7.36	134.94	121.70
1	B	468	ASN	C-N-CA	7.36	134.94	121.70
1	C	468	ASN	CA-C-N	7.14	134.56	121.70
1	C	468	ASN	C-N-CA	7.14	134.56	121.70
1	A	380	ASP	CA-CB-CG	6.85	119.45	112.60
1	A	322	ASN	CA-C-N	6.48	131.65	121.99
1	A	322	ASN	C-N-CA	6.48	131.65	121.99
1	B	416	VAL	N-CA-CB	-6.13	102.17	112.47
1	A	416	VAL	N-CA-CB	-6.06	102.26	112.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	468	ASN	N-CA-C	6.02	119.29	109.24
1	C	422	GLY	CA-C-N	5.97	129.35	120.87
1	C	422	GLY	C-N-CA	5.97	129.35	120.87
1	B	355	THR	CB-CA-C	5.97	119.70	111.23
1	A	355	THR	CB-CA-C	5.96	119.69	111.23
1	C	463	ILE	N-CA-CB	5.87	121.08	111.45
1	A	468	ASN	N-CA-C	5.78	118.89	109.24
2	D	101	ARG	CA-C-N	5.77	128.01	120.28
2	D	101	ARG	C-N-CA	5.77	128.01	120.28
1	A	463	ILE	N-CA-CB	5.70	120.81	111.45
1	B	463	ILE	N-CA-CB	5.66	120.73	111.45
1	B	468	ASN	N-CA-C	5.64	118.66	109.24
1	B	409	LEU	N-CA-C	-5.55	104.63	111.40
1	C	355	THR	CB-CA-C	5.53	119.09	111.23
1	B	332	MET	N-CA-C	5.52	117.10	107.49
1	A	422	GLY	CA-C-N	5.49	128.67	120.87
1	A	422	GLY	C-N-CA	5.49	128.67	120.87
2	E	101	ARG	CA-C-N	5.44	127.51	120.44
2	E	101	ARG	C-N-CA	5.44	127.51	120.44
1	C	323	ARG	CB-CA-C	-5.39	101.35	110.19
1	A	407	ASP	CA-CB-CG	5.25	117.85	112.60
1	C	449	THR	CB-CA-C	5.20	118.40	109.51
1	A	321	ASN	N-CA-C	5.18	120.46	114.04
1	A	409	LEU	N-CA-C	-5.18	105.72	111.36
1	B	322	ASN	N-CA-C	-5.16	104.30	111.52
1	A	455	GLN	CB-CG-CD	-5.15	103.84	112.60
2	F	101	ARG	CA-C-N	5.12	127.15	120.28
2	F	101	ARG	C-N-CA	5.12	127.15	120.28
1	A	451	THR	CA-C-N	5.11	124.83	119.92
1	A	451	THR	C-N-CA	5.11	124.83	119.92
1	B	318	ASP	CA-CB-CG	5.03	117.63	112.60
1	B	323	ARG	N-CA-C	5.02	118.82	111.04

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	1294	0	1232	28	0
1	B	1294	0	1232	31	0
1	C	1294	0	1232	29	0
2	D	798	0	775	11	0
2	E	798	0	775	11	0
2	F	798	0	775	11	0
All	All	6276	0	6021	105	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 9.

All (105) 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:B:318:ASP:HB3	1:B:323:ARG:HB2	1.30	1.12
1:A:318:ASP:HB3	1:A:323:ARG:HB2	1.34	1.09
1:C:318:ASP:HB3	1:C:323:ARG:HB2	1.32	1.07
1:B:406:ILE:HD12	1:C:359:MET:HE3	1.48	0.95
1:A:359:MET:HE3	1:C:406:ILE:HD12	1.47	0.95
1:A:406:ILE:HD12	1:B:359:MET:HE3	1.60	0.83
1:B:312:ARG:HB3	1:C:325:GLN:HB3	1.64	0.80
2:D:39:ARG:HG2	2:D:127:ILE:HD12	1.68	0.75
1:A:325:GLN:HB3	1:C:312:ARG:HB3	1.69	0.73
1:A:333:ARG:NH1	1:A:469:VAL:HG11	2.04	0.71
1:A:312:ARG:HB3	1:B:325:GLN:HB3	1.72	0.71
1:B:333:ARG:NH1	1:B:469:VAL:HG11	2.05	0.71
1:C:333:ARG:NH1	1:C:469:VAL:HG11	2.06	0.71
1:B:333:ARG:HH12	1:B:469:VAL:HG11	1.55	0.70
1:A:333:ARG:HH12	1:A:469:VAL:HG11	1.57	0.69
1:C:333:ARG:HH12	1:C:469:VAL:HG11	1.59	0.66
1:A:322:ASN:ND2	1:C:308:LEU:O	2.30	0.65
1:B:315:LEU:HD11	1:C:315:LEU:HD22	1.81	0.62
1:A:318:ASP:HB3	1:A:323:ARG:CB	2.22	0.61
1:A:377:ILE:HG12	1:A:456:VAL:HG21	1.83	0.61
1:C:359:MET:HG3	1:C:366:VAL:HB	1.82	0.60
1:B:311:TYR:CD1	1:C:324:VAL:HB	2.36	0.60
2:D:39:ARG:HB3	2:D:129:LEU:HD11	1.83	0.59
1:B:367:LEU:HB2	1:B:463:ILE:HD12	1.86	0.58
1:B:317:LEU:HD23	1:B:324:VAL:CG2	2.34	0.57
1:A:367:LEU:HB2	1:A:463:ILE:HD12	1.87	0.57
1:A:333:ARG:HB2	1:A:360:LYS:HB2	1.87	0.57
1:C:318:ASP:HB3	1:C:323:ARG:CB	2.22	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:412:THR:HG22	1:B:463:ILE:HG23	1.87	0.56
1:B:369:PHE:HE1	1:B:463:ILE:HD11	1.70	0.56
1:B:316:GLU:O	1:B:324:VAL:HA	2.05	0.56
2:D:104:THR:HG23	2:D:127:ILE:HA	1.88	0.56
2:E:39:ARG:HB2	2:E:129:LEU:HD11	1.89	0.55
2:F:104:THR:HG23	2:F:127:ILE:HA	1.89	0.55
1:B:419:LEU:HD22	1:B:424:ARG:HG2	1.87	0.55
1:C:333:ARG:HB2	1:C:360:LYS:HB2	1.89	0.55
1:C:367:LEU:HB2	1:C:463:ILE:HD12	1.88	0.55
1:B:377:ILE:HG12	1:B:456:VAL:HG21	1.88	0.54
1:C:412:THR:HG22	1:C:463:ILE:HG23	1.90	0.54
1:A:369:PHE:HE1	1:A:463:ILE:HD11	1.73	0.54
1:B:333:ARG:HB2	1:B:360:LYS:HB2	1.91	0.53
2:E:104:THR:HG23	2:E:127:ILE:HA	1.89	0.53
1:C:338:THR:HG23	1:C:355:THR:HB	1.91	0.52
2:D:39:ARG:CG	2:D:127:ILE:HD12	2.38	0.52
2:F:39:ARG:HB2	2:F:129:LEU:HD11	1.91	0.52
1:C:418:PHE:HE2	1:C:450:TYR:HA	1.75	0.52
2:F:48:LEU:HD21	2:F:126:LEU:HD13	1.92	0.52
1:B:317:LEU:HD23	1:B:324:VAL:HG22	1.93	0.51
1:B:407:ASP:OD2	1:B:434:SER:HB2	2.11	0.51
1:A:412:THR:HG21	1:A:462:THR:O	2.10	0.51
1:B:396:GLN:HE21	2:E:110:MET:HG2	1.75	0.51
2:E:48:LEU:HD21	2:E:126:LEU:HD13	1.91	0.51
1:C:369:PHE:HE1	1:C:463:ILE:HD11	1.76	0.51
1:A:338:THR:HG23	1:A:355:THR:HB	1.93	0.50
1:B:338:THR:HG23	1:B:355:THR:HB	1.92	0.50
1:A:317:LEU:HD23	1:A:324:VAL:HG22	1.93	0.49
1:C:377:ILE:HG12	1:C:456:VAL:HG21	1.94	0.49
2:F:74:CYS:HB2	2:F:79:ILE:HD13	1.95	0.49
1:C:418:PHE:CE2	1:C:450:TYR:HA	2.48	0.48
2:F:47:LYS:HB2	2:F:95:THR:HG23	1.95	0.48
1:C:406:ILE:O	1:C:409:LEU:HG	2.13	0.48
2:D:48:LEU:HD21	2:D:126:LEU:HD13	1.95	0.48
2:E:47:LYS:HB2	2:E:95:THR:HG23	1.95	0.48
1:A:406:ILE:CD1	1:B:359:MET:HE3	2.37	0.48
1:A:412:THR:HG22	1:A:463:ILE:HG23	1.95	0.48
2:F:62:TRP:HB2	2:F:74:CYS:HB3	1.95	0.47
2:D:47:LYS:HB2	2:D:95:THR:HG23	1.95	0.47
1:A:417:GLN:NE2	1:A:424:ARG:HB3	2.29	0.47
2:F:106:THR:HG21	2:F:123:LYS:HE3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:318:ASP:CB	1:B:323:ARG:HB2	2.22	0.47
2:F:50:CYS:HB2	2:F:62:TRP:CZ2	2.50	0.46
2:D:50:CYS:HB2	2:D:62:TRP:CZ2	2.51	0.46
1:A:311:TYR:HD2	1:A:317:LEU:HB2	1.81	0.46
2:E:106:THR:HG21	2:E:123:LYS:HE3	1.97	0.46
1:A:321:ASN:HB3	1:A:323:ARG:CG	2.47	0.45
1:C:342:GLN:HB2	1:C:384:VAL:HB	1.98	0.45
2:D:50:CYS:HB2	2:D:62:TRP:HZ2	1.82	0.45
2:E:39:ARG:HB3	2:E:127:ILE:HD12	1.99	0.45
2:E:50:CYS:HB2	2:E:62:TRP:HZ2	1.82	0.45
2:D:106:THR:HG21	2:D:123:LYS:HE3	1.97	0.45
1:B:342:GLN:HB2	1:B:384:VAL:HB	1.99	0.44
1:B:359:MET:HG3	1:B:366:VAL:HB	1.98	0.44
2:F:64:PHE:CZ	2:F:66:GLN:HB2	2.52	0.44
1:B:418:PHE:HB3	1:B:453:HIS:HB3	1.99	0.44
1:B:311:TYR:CE1	1:C:324:VAL:HB	2.53	0.44
2:E:50:CYS:HB2	2:E:62:TRP:CZ2	2.51	0.44
1:A:359:MET:HG3	1:A:366:VAL:HB	1.99	0.44
1:A:311:TYR:CD2	1:A:317:LEU:HB2	2.53	0.44
2:F:50:CYS:HB2	2:F:62:TRP:HZ2	1.81	0.44
1:A:359:MET:HE3	1:C:406:ILE:CD1	2.31	0.44
2:E:64:PHE:CZ	2:E:66:GLN:HB2	2.53	0.43
2:F:39:ARG:HB3	2:F:127:ILE:HD12	1.98	0.43
1:A:416:VAL:HG13	1:A:456:VAL:HG13	1.99	0.43
1:A:342:GLN:HB2	1:A:384:VAL:HB	2.00	0.43
1:B:428:PHE:CE2	1:B:449:THR:HG23	2.54	0.43
1:C:417:GLN:HA	1:C:425:ILE:O	2.18	0.43
2:D:64:PHE:CZ	2:D:66:GLN:HB2	2.53	0.43
1:B:469:VAL:HG13	2:E:59:ARG:HH12	1.83	0.42
1:C:311:TYR:CD2	1:C:317:LEU:HB2	2.55	0.42
1:C:321:ASN:HB3	1:C:323:ARG:CG	2.48	0.42
1:B:317:LEU:HD23	1:B:324:VAL:HG23	2.00	0.41
2:D:72:LEU:HB3	2:D:80:THR:HG21	2.02	0.41
1:A:312:ARG:NH1	1:B:325:GLN:HE21	2.18	0.41
1:A:322:ASN:CG	1:C:309:PRO:HA	2.45	0.41
1:C:418:PHE:HD2	1:C:451:THR:HG22	1.86	0.41

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	160/165 (97%)	150 (94%)	10 (6%)	0	100	100
1	B	160/165 (97%)	149 (93%)	9 (6%)	2 (1%)	9	40
1	C	160/165 (97%)	150 (94%)	10 (6%)	0	100	100
2	D	100/104 (96%)	98 (98%)	2 (2%)	0	100	100
2	E	100/104 (96%)	97 (97%)	3 (3%)	0	100	100
2	F	100/104 (96%)	97 (97%)	3 (3%)	0	100	100
All	All	780/807 (97%)	741 (95%)	37 (5%)	2 (0%)	36	68

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	320	ALA
1	B	324	VAL

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	141/144 (98%)	126 (89%)	15 (11%)	6	27
1	B	141/144 (98%)	128 (91%)	13 (9%)	8	33
1	C	141/144 (98%)	125 (89%)	16 (11%)	5	24
2	D	93/94 (99%)	84 (90%)	9 (10%)	8	32
2	E	93/94 (99%)	83 (89%)	10 (11%)	6	27

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	F	93/94 (99%)	84 (90%)	9 (10%)	8	32
All	All	702/714 (98%)	630 (90%)	72 (10%)	7	28

All (72) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	310	THR
1	A	317	LEU
1	A	323	ARG
1	A	325	GLN
1	A	349	SER
1	A	359	MET
1	A	371	GLN
1	A	376	SER
1	A	382	LYS
1	A	389	SER
1	A	393	SER
1	A	419	LEU
1	A	462	THR
1	A	463	ILE
1	A	468	ASN
1	B	310	THR
1	B	323	ARG
1	B	325	GLN
1	B	349	SER
1	B	359	MET
1	B	371	GLN
1	B	376	SER
1	B	389	SER
1	B	393	SER
1	B	416	VAL
1	B	462	THR
1	B	463	ILE
1	B	468	ASN
1	C	310	THR
1	C	317	LEU
1	C	323	ARG
1	C	325	GLN
1	C	349	SER
1	C	359	MET
1	C	371	GLN
1	C	376	SER

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Mol	Chain	Res	Type
1	C	389	SER
1	C	393	SER
1	C	409	LEU
1	C	416	VAL
1	C	434	SER
1	C	462	THR
1	C	463	ILE
1	C	468	ASN
2	D	40	ILE
2	D	53	SER
2	D	69	THR
2	D	72	LEU
2	D	77	ASN
2	D	95	THR
2	D	98	SER
2	D	99	VAL
2	D	127	ILE
2	E	40	ILE
2	E	53	SER
2	E	69	THR
2	E	72	LEU
2	E	73	VAL
2	E	77	ASN
2	E	84	GLU
2	E	95	THR
2	E	98	SER
2	E	127	ILE
2	F	40	ILE
2	F	53	SER
2	F	69	THR
2	F	72	LEU
2	F	77	ASN
2	F	84	GLU
2	F	95	THR
2	F	98	SER
2	F	127	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	325	GLN
1	A	342	GLN

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Mol	Chain	Res	Type
1	A	347	GLN
1	A	353	ASN
1	A	386	ASN
1	B	325	GLN
1	B	342	GLN
1	B	353	ASN
1	B	386	ASN
1	C	325	GLN
1	C	340	GLN
1	C	342	GLN
1	C	347	GLN
1	C	371	GLN
1	C	386	ASN
2	D	44	ASN
2	E	44	ASN
2	F	44	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](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

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	162/165 (98%)	-0.06	2 (1%) 76 58	26, 49, 100, 116	0
1	B	162/165 (98%)	0.07	1 (0%) 85 73	28, 57, 97, 120	0
1	C	162/165 (98%)	0.36	3 (1%) 66 46	36, 70, 100, 116	0
2	D	102/104 (98%)	0.45	4 (3%) 43 27	51, 72, 101, 104	0
2	E	102/104 (98%)	1.30	16 (15%) 5 4	91, 120, 144, 155	0
2	F	102/104 (98%)	1.35	20 (19%) 3 2	118, 138, 160, 168	0
All	All	792/807 (98%)	0.48	46 (5%) 29 18	26, 71, 147, 168	0

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	469	VAL	4.3
2	E	50	CYS	3.8
1	A	469	VAL	3.7
2	E	124	VAL	3.5
2	E	127	ILE	3.5
1	B	469	VAL	3.3
2	E	48	LEU	3.2
2	E	46	VAL	3.1
2	F	123	LYS	3.0
2	F	59	ARG	3.0
2	F	72	LEU	2.8
2	E	62	TRP	2.8
2	D	50	CYS	2.7
2	F	62	TRP	2.7
2	E	122	VAL	2.7
2	F	99	VAL	2.6
2	E	96	PHE	2.5
2	F	124	VAL	2.5
2	F	30	THR	2.5

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Mol	Chain	Res	Type	RSRZ
2	E	38	VAL	2.5
2	F	126	LEU	2.4
1	C	438	ASP	2.4
2	F	67	GLY	2.4
2	F	94	ILE	2.3
2	E	126	LEU	2.3
2	F	52	TYR	2.3
2	F	50	CYS	2.3
2	F	71	ARG	2.3
2	F	106	THR	2.2
2	E	107	TYR	2.2
2	E	125	LYS	2.2
2	D	34	SER	2.2
2	F	112	SER	2.2
2	D	30	THR	2.2
2	F	40	ILE	2.2
2	D	117	ASN	2.2
2	E	109	CYS	2.2
2	F	110	MET	2.2
2	F	76	ASN	2.2
2	E	105	GLY	2.2
1	A	324	VAL	2.1
2	E	111	VAL	2.1
2	E	90	LEU	2.1
1	C	422	GLY	2.0
2	F	116	GLY	2.0
2	F	46	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.