Full wwPDB X-ray Structure Validation Report ⓘ

Sep 11, 2023 – 01:32 AM EDT

PDB ID	:	4JGS
Title	:	Crystal structure of the xmrv tm retroviral fusion core
Authors	:	Cook, J.D.; Aydin, H.; Lee, J.E.
Deposited on	:	2013-03-02
Resolution	:	2.20 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:

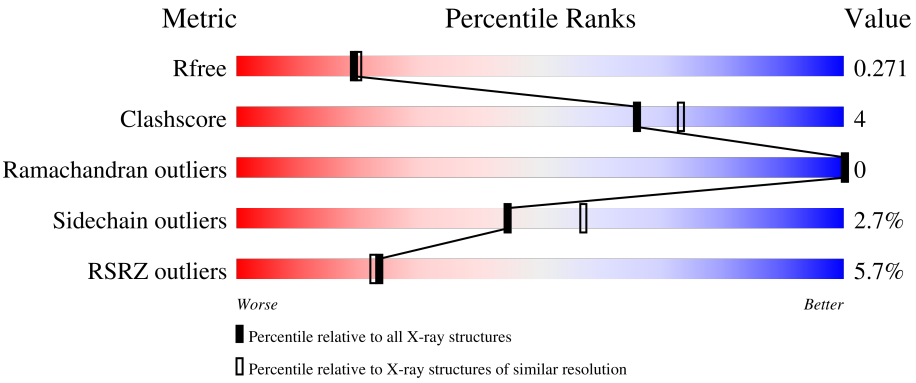
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 2.20 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}	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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 <=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	105	4% 73% 22%
1	B	105	2% 74% 22%
1	C	105	4% 68% 16% 16%
1	D	105	6% 70% 10% 19%
1	E	105	3% 75% 20%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	105	9% 69% 8% 24%
1	G	105	6% 76% 9% 14%
1	H	105	7% 73% 6% 20%
1	I	105	2% 70% 7% 22%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 6052 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 MLV-related proviral Env polyprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	82	Total	C	N	O	S	0	0	0
			634	395	114	122	3			
1	B	82	Total	C	N	O	S	0	0	0
			620	388	110	119	3			
1	C	88	Total	C	N	O	S	0	0	0
			668	414	123	128	3			
1	D	85	Total	C	N	O	S	0	0	0
			645	402	114	126	3			
1	E	84	Total	C	N	O	S	0	0	0
			633	396	114	120	3			
1	F	80	Total	C	N	O	S	0	0	0
			606	380	107	116	3			
1	G	90	Total	C	N	O	S	0	0	0
			693	432	126	132	3			
1	H	84	Total	C	N	O	S	0	0	0
			633	396	112	122	3			
1	I	82	Total	C	N	O	S	0	0	0
			616	385	109	119	3			

There are 99 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	464	SER	-	expression tag	UNP P10404
A	465	SER	-	expression tag	UNP P10404
A	466	GLY	-	expression tag	UNP P10404
A	467	LEU	-	expression tag	UNP P10404
A	468	VAL	-	expression tag	UNP P10404
A	469	GLY	-	expression tag	UNP P10404
A	470	SER	-	expression tag	UNP P10404
A	471	GLY	-	expression tag	UNP P10404
A	472	THR	-	expression tag	UNP P10404
A	538	SER	CYS	conflict	UNP P10404
A	563	ARG	LYS	conflict	UNP P10404

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	464	SER	-	expression tag	UNP P10404
B	465	SER	-	expression tag	UNP P10404
B	466	GLY	-	expression tag	UNP P10404
B	467	LEU	-	expression tag	UNP P10404
B	468	VAL	-	expression tag	UNP P10404
B	469	GLY	-	expression tag	UNP P10404
B	470	SER	-	expression tag	UNP P10404
B	471	GLY	-	expression tag	UNP P10404
B	472	THR	-	expression tag	UNP P10404
B	538	SER	CYS	conflict	UNP P10404
B	563	ARG	LYS	conflict	UNP P10404
C	464	SER	-	expression tag	UNP P10404
C	465	SER	-	expression tag	UNP P10404
C	466	GLY	-	expression tag	UNP P10404
C	467	LEU	-	expression tag	UNP P10404
C	468	VAL	-	expression tag	UNP P10404
C	469	GLY	-	expression tag	UNP P10404
C	470	SER	-	expression tag	UNP P10404
C	471	GLY	-	expression tag	UNP P10404
C	472	THR	-	expression tag	UNP P10404
C	538	SER	CYS	conflict	UNP P10404
C	563	ARG	LYS	conflict	UNP P10404
D	464	SER	-	expression tag	UNP P10404
D	465	SER	-	expression tag	UNP P10404
D	466	GLY	-	expression tag	UNP P10404
D	467	LEU	-	expression tag	UNP P10404
D	468	VAL	-	expression tag	UNP P10404
D	469	GLY	-	expression tag	UNP P10404
D	470	SER	-	expression tag	UNP P10404
D	471	GLY	-	expression tag	UNP P10404
D	472	THR	-	expression tag	UNP P10404
D	538	SER	CYS	conflict	UNP P10404
D	563	ARG	LYS	conflict	UNP P10404
E	464	SER	-	expression tag	UNP P10404
E	465	SER	-	expression tag	UNP P10404
E	466	GLY	-	expression tag	UNP P10404
E	467	LEU	-	expression tag	UNP P10404
E	468	VAL	-	expression tag	UNP P10404
E	469	GLY	-	expression tag	UNP P10404
E	470	SER	-	expression tag	UNP P10404
E	471	GLY	-	expression tag	UNP P10404
E	472	THR	-	expression tag	UNP P10404

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
E	538	SER	CYS	conflict	UNP P10404
E	563	ARG	LYS	conflict	UNP P10404
F	464	SER	-	expression tag	UNP P10404
F	465	SER	-	expression tag	UNP P10404
F	466	GLY	-	expression tag	UNP P10404
F	467	LEU	-	expression tag	UNP P10404
F	468	VAL	-	expression tag	UNP P10404
F	469	GLY	-	expression tag	UNP P10404
F	470	SER	-	expression tag	UNP P10404
F	471	GLY	-	expression tag	UNP P10404
F	472	THR	-	expression tag	UNP P10404
F	538	SER	CYS	conflict	UNP P10404
F	563	ARG	LYS	conflict	UNP P10404
G	464	SER	-	expression tag	UNP P10404
G	465	SER	-	expression tag	UNP P10404
G	466	GLY	-	expression tag	UNP P10404
G	467	LEU	-	expression tag	UNP P10404
G	468	VAL	-	expression tag	UNP P10404
G	469	GLY	-	expression tag	UNP P10404
G	470	SER	-	expression tag	UNP P10404
G	471	GLY	-	expression tag	UNP P10404
G	472	THR	-	expression tag	UNP P10404
G	538	SER	CYS	conflict	UNP P10404
G	563	ARG	LYS	conflict	UNP P10404
H	464	SER	-	expression tag	UNP P10404
H	465	SER	-	expression tag	UNP P10404
H	466	GLY	-	expression tag	UNP P10404
H	467	LEU	-	expression tag	UNP P10404
H	468	VAL	-	expression tag	UNP P10404
H	469	GLY	-	expression tag	UNP P10404
H	470	SER	-	expression tag	UNP P10404
H	471	GLY	-	expression tag	UNP P10404
H	472	THR	-	expression tag	UNP P10404
H	538	SER	CYS	conflict	UNP P10404
H	563	ARG	LYS	conflict	UNP P10404
I	464	SER	-	expression tag	UNP P10404
I	465	SER	-	expression tag	UNP P10404
I	466	GLY	-	expression tag	UNP P10404
I	467	LEU	-	expression tag	UNP P10404
I	468	VAL	-	expression tag	UNP P10404
I	469	GLY	-	expression tag	UNP P10404
I	470	SER	-	expression tag	UNP P10404

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
I	471	GLY	-	expression tag	UNP P10404
I	472	THR	-	expression tag	UNP P10404
I	538	SER	CYS	conflict	UNP P10404
I	563	ARG	LYS	conflict	UNP P10404

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Cl 1 1	0	0
2	B	1	Total Cl 1 1	0	0
2	C	1	Total Cl 1 1	0	0

- Molecule 3 is water.

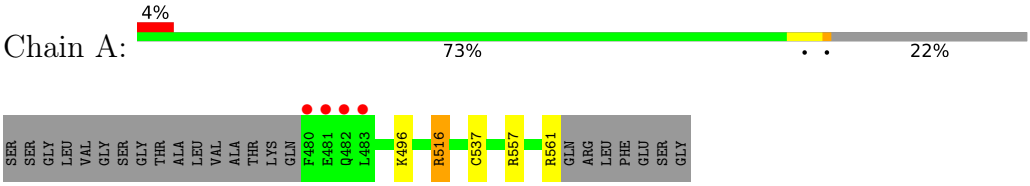
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	33	Total O 33 33	0	0
3	B	30	Total O 30 30	0	0
3	C	39	Total O 39 39	0	0
3	D	32	Total O 32 32	0	0
3	E	33	Total O 33 33	0	0
3	F	31	Total O 31 31	0	0
3	G	33	Total O 33 33	0	0
3	H	34	Total O 34 34	0	0
3	I	36	Total O 36 36	0	0

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.

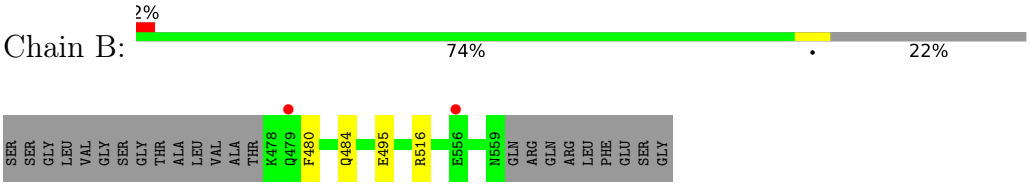
• Molecule 1: MLV-related proviral Env polyprotein

Chain A:



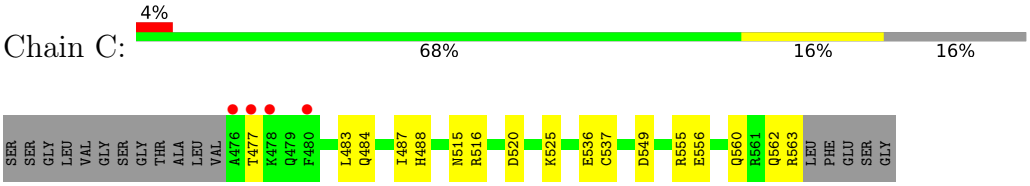
• Molecule 1: MLV-related proviral Env polyprotein

Chain B:



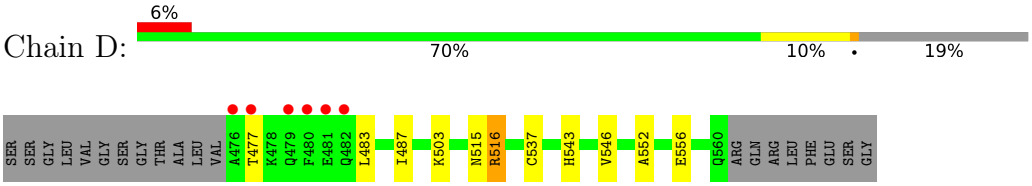
• Molecule 1: MLV-related proviral Env polyprotein

Chain C:



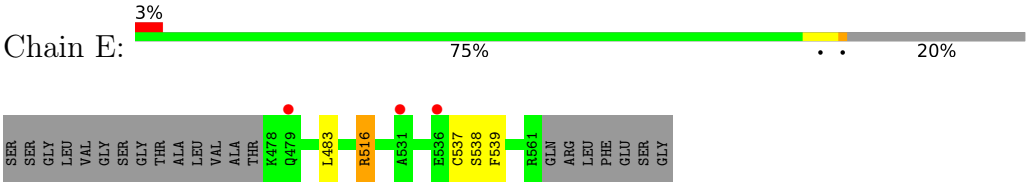
• Molecule 1: MLV-related proviral Env polyprotein

Chain D:



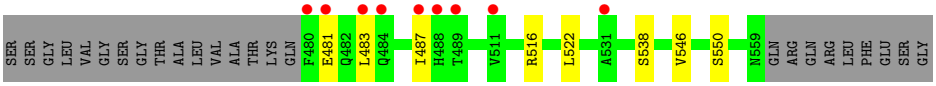
• Molecule 1: MLV-related proviral Env polyprotein

Chain E:



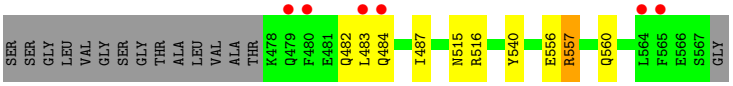
• Molecule 1: MLV-related proviral Env polyprotein

Chain F:



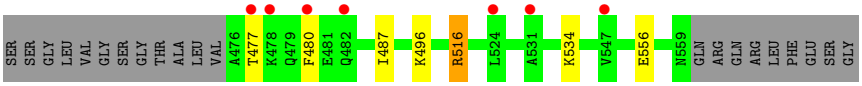
• Molecule 1: MLV-related proviral Env polyprotein

Chain G:



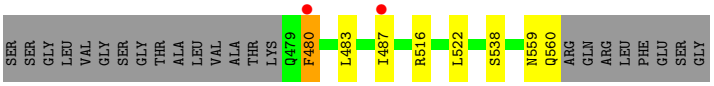
• Molecule 1: MLV-related proviral Env polyprotein

Chain H:



• Molecule 1: MLV-related proviral Env polyprotein

Chain I:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	99.97Å 148.42Å 58.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.58 – 2.20 45.75 – 2.20	Depositor EDS
% Data completeness (in resolution range)	(Not available) (47.58-2.20) 99.9 (45.75-2.20)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.20 (at 2.20Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.214 , 0.266 0.216 , 0.271	Depositor DCC
R_{free} test set	1767 reflections (3.95%)	wwPDB-VP
Wilson B-factor (Å^2)	40.2	Xtriage
Anisotropy	0.058	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 39.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.54$, $< L^2 > = 0.38$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	6052	wwPDB-VP
Average B, all atoms (Å^2)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.91% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: CL

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	0.65	0/639	0.74	2/856 (0.2%)
1	B	0.63	0/625	0.73	2/839 (0.2%)
1	C	0.65	0/673	0.83	3/904 (0.3%)
1	D	0.63	0/650	0.73	1/873 (0.1%)
1	E	0.66	0/638	0.67	1/856 (0.1%)
1	F	0.65	0/611	0.70	0/820
1	G	0.65	0/699	0.87	4/938 (0.4%)
1	H	0.67	0/638	0.77	2/857 (0.2%)
1	I	0.63	0/621	0.70	0/835
All	All	0.64	0/5794	0.75	15/7778 (0.2%)

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	H	516	ARG	NE-CZ-NH2	-9.46	115.57	120.30
1	C	516	ARG	NE-CZ-NH2	-8.90	115.85	120.30
1	B	516	ARG	NE-CZ-NH2	-8.78	115.91	120.30
1	G	557	ARG	NE-CZ-NH1	8.07	124.33	120.30
1	D	516	ARG	NE-CZ-NH2	-7.91	116.34	120.30
1	C	516	ARG	NE-CZ-NH1	7.64	124.12	120.30
1	G	516	ARG	NE-CZ-NH2	-7.59	116.51	120.30
1	A	516	ARG	NE-CZ-NH2	-7.55	116.53	120.30
1	B	516	ARG	NE-CZ-NH1	7.15	123.88	120.30
1	G	557	ARG	NE-CZ-NH2	-7.09	116.76	120.30
1	H	516	ARG	NE-CZ-NH1	7.00	123.80	120.30
1	G	516	ARG	NE-CZ-NH1	6.86	123.73	120.30
1	C	555	ARG	NE-CZ-NH1	-6.16	117.22	120.30
1	A	516	ARG	NE-CZ-NH1	5.05	122.83	120.30
1	E	516	ARG	NE-CZ-NH2	-5.05	117.77	120.30

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	634	0	643	2	0
1	B	620	0	622	3	0
1	C	668	0	665	8	0
1	D	645	0	646	12	0
1	E	633	0	633	4	0
1	F	606	0	612	6	0
1	G	693	0	687	11	0
1	H	633	0	636	8	0
1	I	616	0	611	6	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
3	A	33	0	0	0	0
3	B	30	0	0	1	0
3	C	39	0	0	1	0
3	D	32	0	0	1	0
3	E	33	0	0	1	0
3	F	31	0	0	0	0
3	G	33	0	0	1	0
3	H	34	0	0	2	0
3	I	36	0	0	0	0
All	All	6052	0	5755	46	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 4.

All (46) 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:536:GLU:OE2	1:G:557:ARG:NH2	1.95	0.99
1:G:482:GLN:O	3:G:622:HOH:O	1.96	0.81

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:520:ASP:OD2	3:C:718:HOH:O	2.01	0.79
1:H:534:LYS:O	3:H:613:HOH:O	2.05	0.75
1:C:536:GLU:CD	1:G:557:ARG:HH22	1.92	0.74
1:G:540:TYR:O	1:H:556:GLU:HG3	1.88	0.73
1:G:540:TYR:O	1:H:556:GLU:CG	2.44	0.66
1:C:556:GLU:O	1:C:560:GLN:HG2	1.95	0.66
1:F:483:LEU:HG	1:F:487:ILE:CD1	2.28	0.63
1:D:552:ALA:O	1:D:556:GLU:HG3	1.99	0.63
1:B:484:GLN:OE1	1:I:483:LEU:HD13	1.99	0.61
1:B:495:GLU:OE1	3:B:723:HOH:O	2.17	0.58
1:I:480:PHE:CD2	1:I:480:PHE:C	2.77	0.57
1:D:483:LEU:HD21	1:D:487:ILE:CD1	2.36	0.54
1:D:503:LYS:NZ	3:D:631:HOH:O	2.39	0.54
1:I:516:ARG:NH2	1:I:538:SER:O	2.41	0.53
1:F:483:LEU:HG	1:F:487:ILE:HD12	1.91	0.53
1:F:483:LEU:HG	1:F:487:ILE:HD11	1.90	0.53
1:E:539:PHE:O	3:E:601:HOH:O	2.19	0.52
1:E:483:LEU:CD2	1:G:484:GLN:HG2	2.40	0.52
1:D:483:LEU:HD12	1:H:480:PHE:CE1	2.44	0.52
1:F:546:VAL:O	1:F:550:SER:HB3	2.10	0.51
1:I:559:ASN:O	1:I:560:GLN:HG2	2.10	0.51
1:D:483:LEU:CD2	1:D:487:ILE:HD12	2.40	0.51
1:C:487:ILE:HD13	1:H:487:ILE:HD13	1.92	0.51
1:D:483:LEU:HD21	1:D:487:ILE:HD11	1.92	0.51
1:D:483:LEU:CD2	1:D:487:ILE:CD1	2.90	0.49
1:G:483:LEU:O	1:G:487:ILE:HD12	2.12	0.49
1:F:522:LEU:HD13	1:I:522:LEU:HD13	1.94	0.49
1:D:515:ASN:OD1	1:H:516:ARG:HD3	2.12	0.49
1:I:483:LEU:HG	1:I:487:ILE:HD12	1.95	0.48
1:B:480:PHE:O	1:B:484:GLN:HG3	2.14	0.48
1:D:483:LEU:C	1:D:483:LEU:HD23	2.35	0.47
1:A:516:ARG:HD3	1:G:515:ASN:OD1	2.16	0.46
1:D:483:LEU:HD23	1:D:483:LEU:O	2.16	0.45
1:A:557:ARG:O	1:A:561:ARG:HG3	2.17	0.45
1:F:516:ARG:NH2	1:F:538:SER:O	2.50	0.45
1:E:516:ARG:NH2	1:E:538:SER:O	2.50	0.44
1:G:540:TYR:O	1:H:556:GLU:HG2	2.18	0.44
1:C:483:LEU:O	1:C:487:ILE:HG13	2.18	0.43
1:C:515:ASN:OD1	1:D:516:ARG:HD3	2.19	0.43
1:E:483:LEU:HD21	1:G:484:GLN:HG2	2.00	0.42
1:H:556:GLU:HG2	3:H:617:HOH:O	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:488:HIS:NE2	1:C:562:GLN:OE1	2.52	0.42
1:G:556:GLU:OE1	1:G:556:GLU:HA	2.20	0.41
1:D:543:HIS:O	1:D:546:VAL:HG12	2.21	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	80/105 (76%)	79 (99%)	1 (1%)	0	100	100
1	B	80/105 (76%)	79 (99%)	1 (1%)	0	100	100
1	C	86/105 (82%)	86 (100%)	0	0	100	100
1	D	83/105 (79%)	83 (100%)	0	0	100	100
1	E	82/105 (78%)	81 (99%)	1 (1%)	0	100	100
1	F	78/105 (74%)	78 (100%)	0	0	100	100
1	G	88/105 (84%)	88 (100%)	0	0	100	100
1	H	82/105 (78%)	81 (99%)	1 (1%)	0	100	100
1	I	80/105 (76%)	79 (99%)	1 (1%)	0	100	100
All	All	739/945 (78%)	734 (99%)	5 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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	68/86 (79%)	66 (97%)	2 (3%)	42	54
1	B	65/86 (76%)	65 (100%)	0	100	100
1	C	69/86 (80%)	63 (91%)	6 (9%)	10	10
1	D	68/86 (79%)	66 (97%)	2 (3%)	42	54
1	E	65/86 (76%)	64 (98%)	1 (2%)	65	78
1	F	64/86 (74%)	63 (98%)	1 (2%)	62	76
1	G	72/86 (84%)	71 (99%)	1 (1%)	67	80
1	H	66/86 (77%)	64 (97%)	2 (3%)	41	53
1	I	64/86 (74%)	63 (98%)	1 (2%)	62	76
All	All	601/774 (78%)	585 (97%)	16 (3%)	44	57

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	496	LYS
1	A	537	CYS
1	C	477	THR
1	C	484	GLN
1	C	525	LYS
1	C	537	CYS
1	C	549	ASP
1	C	563	ARG
1	D	477	THR
1	D	537	CYS
1	E	537	CYS
1	F	481	GLU
1	G	560	GLN
1	H	477	THR
1	H	496	LYS
1	I	480	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA

There are no RNA molecules 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 monosaccharides in this entry.

5.6 Ligand geometry

Of 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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, 95^{th} 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	82/105 (78%)	0.38	4 (4%)	29	28	18, 28, 51, 56	0
1	B	82/105 (78%)	0.27	2 (2%)	59	56	18, 28, 54, 61	0
1	C	88/105 (83%)	0.40	4 (4%)	33	32	16, 27, 56, 67	0
1	D	85/105 (80%)	0.54	6 (7%)	16	14	15, 29, 60, 75	0
1	E	84/105 (80%)	0.43	3 (3%)	42	41	17, 26, 49, 63	0
1	F	80/105 (76%)	0.60	9 (11%)	5	4	17, 30, 51, 67	0
1	G	90/105 (85%)	0.58	6 (6%)	17	16	18, 27, 59, 64	0
1	H	84/105 (80%)	0.57	7 (8%)	11	10	15, 26, 54, 58	0
1	I	82/105 (78%)	0.37	2 (2%)	59	56	17, 27, 55, 73	0
All	All	757/945 (80%)	0.46	43 (5%)	23	22	15, 28, 57, 75	0

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	476	ALA	7.8
1	D	480	PHE	5.2
1	F	483	LEU	4.9
1	I	480	PHE	4.7
1	G	480	PHE	4.6
1	E	479	GLN	4.3
1	H	524	LEU	4.3
1	G	479	GLN	3.9
1	F	480	PHE	3.5
1	D	482	GLN	3.5
1	F	531	ALA	3.3
1	A	482	GLN	3.3
1	G	483	LEU	3.3
1	C	478	LYS	3.3
1	B	479	GLN	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	480	PHE	3.2
1	D	479	GLN	3.1
1	A	483	LEU	3.1
1	D	481	GLU	3.1
1	E	531	ALA	3.0
1	F	481	GLU	3.0
1	D	477	THR	3.0
1	C	477	THR	2.9
1	G	565	PHE	2.8
1	H	480	PHE	2.8
1	A	480	PHE	2.7
1	H	482	GLN	2.7
1	F	489	THR	2.6
1	H	478	LYS	2.6
1	F	487	ILE	2.5
1	F	484	GLN	2.5
1	G	564	LEU	2.5
1	H	531	ALA	2.4
1	I	487	ILE	2.3
1	H	477	THR	2.3
1	H	547	VAL	2.3
1	G	484	GLN	2.2
1	A	481	GLU	2.2
1	E	536	GLU	2.2
1	F	511	VAL	2.2
1	C	476	ALA	2.1
1	F	488	HIS	2.1
1	B	556	GLU	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 monosaccharides 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, 95^{th} 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(Å^2)	Q<0.9
2	CL	A	601	1/1	0.98	0.16	24,24,24,24	0
2	CL	B	601	1/1	0.99	0.14	23,23,23,23	0
2	CL	C	601	1/1	0.99	0.16	17,17,17,17	0

6.5 Other polymers (i)

There are no such residues in this entry.