



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:00 PM UTC

PDB ID : 4BLP / pdb_00004blp
Title : P4 PROTEIN FROM BACTERIOPHAGE PHI13
Authors : El Omari, K.; Meier, C.; Kainov, D.; Sutton, G.; Grimes, J.M.; Poranen, M.M.; Bamford, D.H.; Tuma, R.; Stuart, D.I.; Mancini, E.J.
Deposited on : 2013-05-04
Resolution : 1.70 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

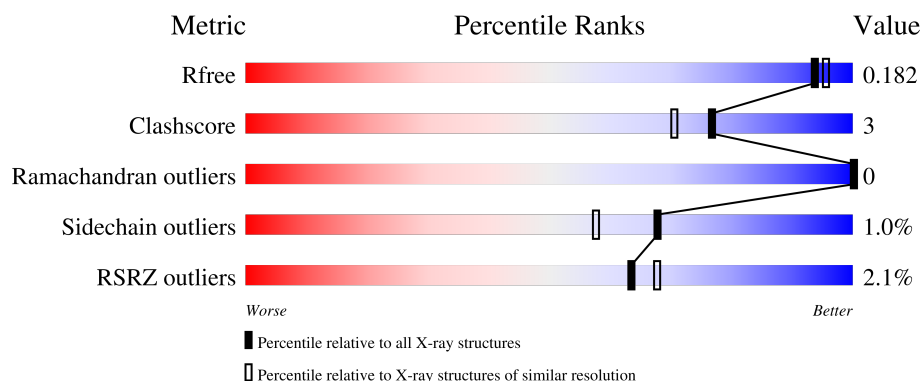
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 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	5551 (1.70-1.70)
Clashscore	190562	5924 (1.70-1.70)
Ramachandran outliers	187476	5846 (1.70-1.70)
Sidechain outliers	187428	5846 (1.70-1.70)
RSRZ outliers	180081	5554 (1.70-1.70)

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	358	2% 70% 6% 24%
1	B	358	3% 70% 6% 25%
1	C	358	% 69% 6% 25%
1	D	358	% 71% 5% 24%
1	E	358	3% 69% 6% 24%

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Mol	Chain	Length	Quality of chain
1	F	358	% 69% 7% 24%

2 Entry composition [i](#)

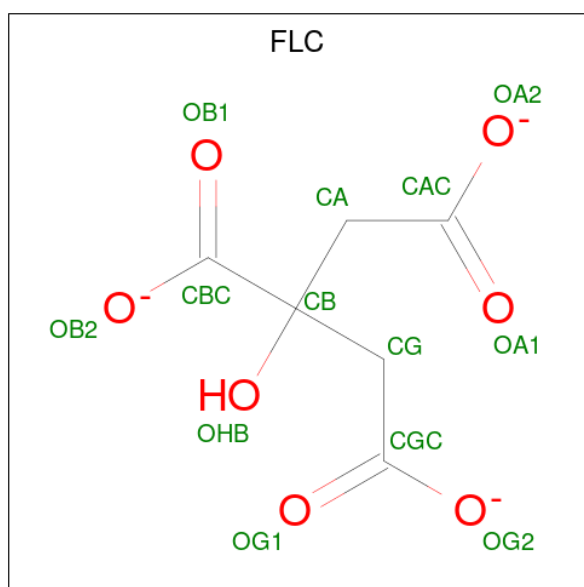
There are 4 unique types of molecules in this entry. The entry contains 13687 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 PACKAGING ENZYME P4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	271	Total	C	N	O	S	0	5	0
			1991	1263	342	380	6			
1	B	270	Total	C	N	O	S	0	12	0
			2019	1282	347	384	6			
1	C	270	Total	C	N	O	S	0	7	0
			1994	1266	343	379	6			
1	D	273	Total	C	N	O	S	0	2	0
			1991	1259	343	383	6			
1	E	271	Total	C	N	O	S	0	8	0
			2007	1275	344	382	6			
1	F	272	Total	C	N	O	S	0	7	0
			2008	1274	343	385	6			

- Molecule 2 is CITRATE ANION (CCD ID: FLC) (formula: $C_6H_5O_7$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			13	6	7		
2	F	1	Total	C	O	0	0
			13	6	7		

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	0
			6	3	3		
3	E	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	293	Total	O	0	0
			293	293		
4	B	263	Total	O	0	0
			263	263		
4	C	250	Total	O	0	0
			250	250		
4	D	293	Total	O	0	0
			293	293		

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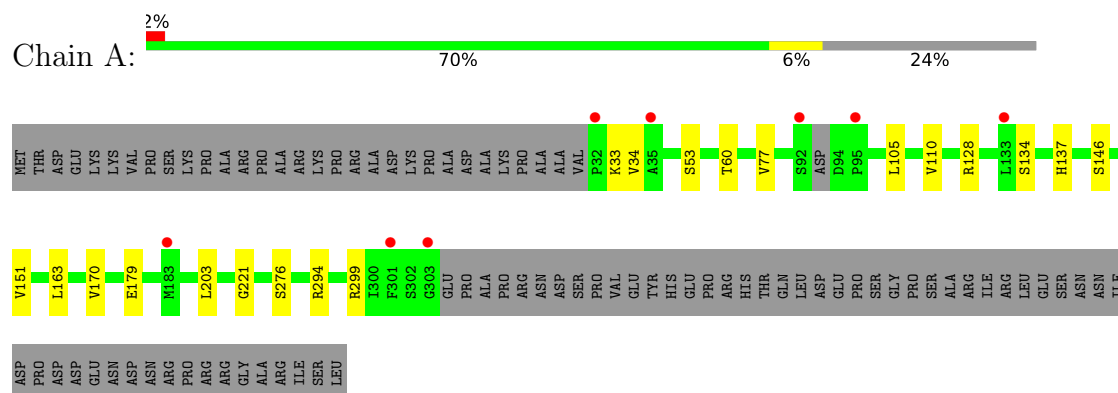
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	E	277	Total 277	O 277	0	0
4	F	251	Total 251	O 251	0	0

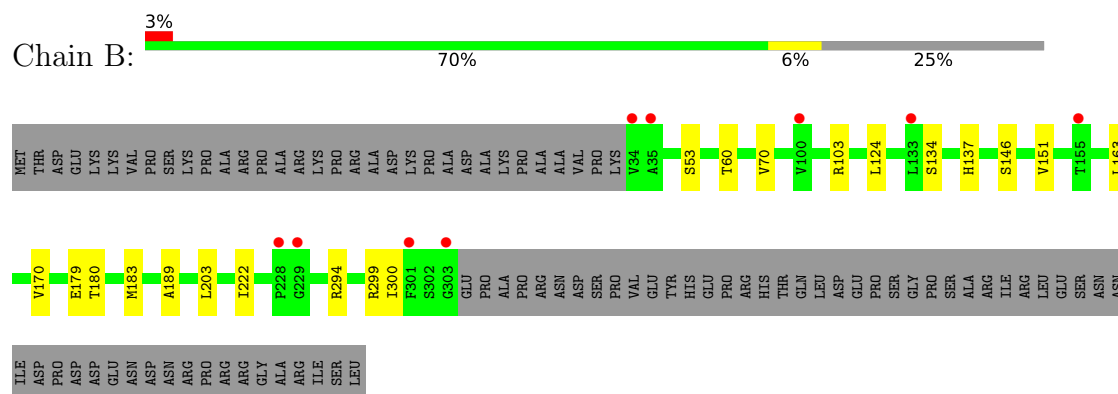
3 Residue-property plots [i](#)

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.

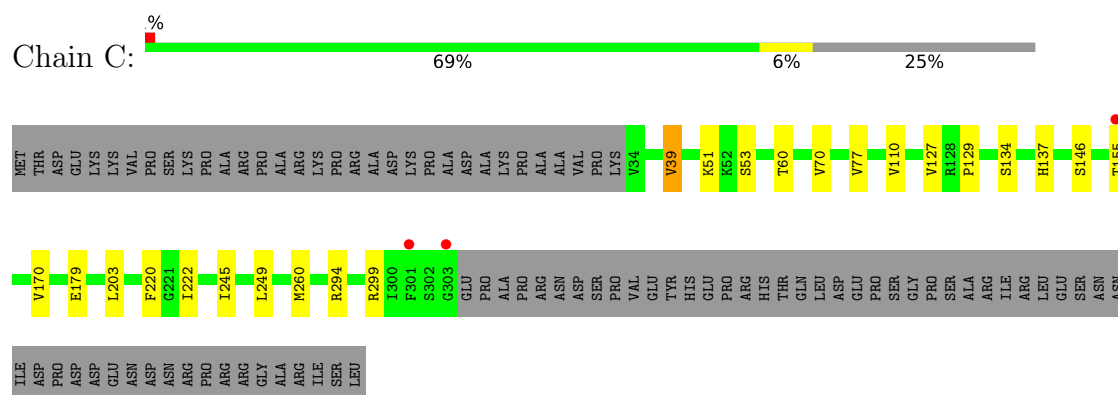
• Molecule 1: PACKAGING ENZYME P4



• Molecule 1: PACKAGING ENZYME P4



• Molecule 1: PACKAGING ENZYME P4



Protein	Residue	Score	Rank
ASP	L163	0.0000	1
ASP	E179	0.0000	2
ARG	T180	0.0000	3
ARG	M183	0.0000	4
ARG	R216	0.0000	5
ALA	T222	0.0000	6
ILE	T223	0.0000	7
SER	P228	0.0000	8
LEU	G229	0.0000	9
ASP	K265	0.0000	10
ASP	T300	0.0000	11
ASP	A306	0.0000	12
ASP	PRO	0.0000	13
ASP	ARG	0.0000	14
ASP	ASN	0.0000	15
ASP	ASP	0.0000	16
ASP	SER	0.0000	17
ASP	PRO	0.0000	18
ASP	VAL	0.0000	19
ASP	GLU	0.0000	20
ASP	TYR	0.0000	21
ASP	HIS	0.0000	22
ASP	GLU	0.0000	23
ASP	PRO	0.0000	24
ASP	ARG	0.0000	25
ASP	HIS	0.0000	26
ASP	THR	0.0000	27
ASP	GLN	0.0000	28
ASP	LEU	0.0000	29
ASP	ASP	0.0000	30
ASP	GLU	0.0000	31
ASP	PRO	0.0000	32
ASP	SER	0.0000	33
ASP	GLY	0.0000	34
ASP	PRO	0.0000	35
ASP	SER	0.0000	36
ASP	ALA	0.0000	37
ASP	ARG	0.0000	38
ASP	ILE	0.0000	39
ASP	ARG	0.0000	40
ASP	LEU	0.0000	41
ASP	GLU	0.0000	42
ASP	SER	0.0000	43
ASP	ASN	0.0000	44
ASP	ASN	0.0000	45
ASP	ILE	0.0000	46
ASP	ASP	0.0000	47
ASP	PRO	0.0000	48
ASP	ASP	0.0000	49
ASP	GLU	0.0000	50
ASP	ASP	0.0000	51
ASP	ASP	0.0000	52
ASP	ASP	0.0000	53
ASP	ASP	0.0000	54
ASP	ASP	0.0000	55
ASP	ASP	0.0000	56
ASP	ASP	0.0000	57
ASP	ASP	0.0000	58
ASP	ASP	0.0000	59
ASP	ASP	0.0000	60
ASP	ASP	0.0000	61
ASP	ASP	0.0000	62
ASP	ASP	0.0000	63
ASP	ASP	0.0000	64
ASP	ASP	0.0000	65
ASP	ASP	0.0000	66
ASP	ASP	0.0000	67
ASP	ASP	0.0000	68
ASP	ASP	0.0000	69
ASP	ASP	0.0000	70
ASP	ASP	0.0000	71
ASP	ASP	0.0000	72
ASP	ASP	0.0000	73
ASP	ASP	0.0000	74
ASP	ASP	0.0000	75
ASP	ASP	0.0000	76
ASP	ASP	0.0000	77
ASP	ASP	0.0000	78
ASP	ASP	0.0000	79
ASP	ASP	0.0000	80
ASP	ASP	0.0000	81
ASP	ASP	0.0000	82
ASP	ASP	0.0000	83
ASP	ASP	0.0000	84
ASP	ASP	0.0000	85
ASP	ASP	0.0000	86
ASP	ASP	0.0000	87
ASP	ASP	0.0000	88
ASP	ASP	0.0000	89
ASP	ASP	0.0000	90
ASP	ASP	0.0000	91
ASP	ASP	0.0000	92
ASP	ASP	0.0000	93
ASP	ASP	0.0000	94
ASP	ASP	0.0000	95
ASP	ASP	0.0000	96
ASP	ASP	0.0000	97
ASP	ASP	0.0000	98

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	97.22Å 116.24Å 149.77Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.85 – 1.70 19.85 – 1.70	Depositor EDS
% Data completeness (in resolution range)	91.1 (19.85-1.70) 99.8 (19.85-1.70)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.04 (at 1.60Å)	Xtriage
Refinement program	BUSTER 2.11.2	Depositor
R, R_{free}	0.163 , 0.188 0.161 , 0.182	Depositor DCC
R_{free} test set	11121 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	21.0	Xtriage
Anisotropy	0.458	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 49.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	13687	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.68% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: FLC, GOL

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	0/2037	0.98	0/2785
1	B	0.89	0/2086	0.97	0/2853
1	C	0.89	0/2046	0.98	1/2799 (0.0%)
1	D	0.93	0/2029	0.99	2/2777 (0.1%)
1	E	0.92	0/2062	1.00	2/2821 (0.1%)
1	F	0.91	0/2061	1.02	0/2821
All	All	0.90	0/12321	0.99	5/16856 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	284	ASN	CA-CB-CG	7.54	120.14	112.60
1	E	263	ASP	CA-CB-CG	6.57	119.17	112.60
1	C	39	VAL	CB-CA-C	6.32	117.44	110.62
1	D	289	VAL	N-CA-C	-5.05	106.76	111.45
1	D	99	PHE	CA-CB-CG	-5.01	108.79	113.80

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	1991	0	2051	13	0
1	B	2019	0	2097	16	0
1	C	1994	0	2062	13	0
1	D	1991	0	2033	9	0
1	E	2007	0	2077	16	0
1	F	2008	0	2065	19	0
2	A	13	0	5	0	0
2	F	13	0	5	0	0
3	B	6	0	8	0	0
3	C	6	0	8	0	0
3	D	6	0	8	0	0
3	E	6	0	8	0	0
4	A	293	0	0	1	0
4	B	263	0	0	2	0
4	C	250	0	0	1	0
4	D	293	0	0	2	0
4	E	277	0	0	2	0
4	F	251	0	0	1	0
All	All	13687	0	12427	72	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 3.

All (72) 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:E:70[B]:VAL:HG11	1:E:193:LEU:HD21	1.68	0.75
1:E:183:MET:SD	1:F:132:SER:HA	2.38	0.63
1:E:183:MET:HE2	1:F:133:LEU:H	1.63	0.63
1:C:77[B]:VAL:HG22	1:C:110:VAL:HG22	1.80	0.62
1:A:128:ARG:HH21	1:F:107:ARG:HH12	1.47	0.62
1:D:55:ARG:NH1	4:D:2036:HOH:O	2.32	0.61
1:A:294:ARG:HD3	1:F:179[B]:GLU:HG2	1.81	0.61
1:E:137:HIS:HE1	1:E:146:SER:OG	1.85	0.59
1:B:179[B]:GLU:HG2	1:C:294:ARG:HD3	1.83	0.59
1:C:137:HIS:HE1	1:C:146:SER:OG	1.86	0.59
1:E:70[B]:VAL:HG23	1:E:238:ALA:HB1	1.85	0.58
1:B:170[B]:VAL:HG11	1:B:203:LEU:HD13	1.86	0.57
1:A:137:HIS:HE1	1:A:146:SER:OG	1.86	0.57
1:E:77[B]:VAL:HG22	1:E:110:VAL:HG22	1.85	0.57
1:C:170[B]:VAL:HG11	1:C:203:LEU:HD13	1.86	0.57
1:B:137:HIS:HE1	1:B:146:SER:OG	1.89	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:170[B]:VAL:HG11	1:A:203:LEU:HD13	1.88	0.56
1:D:137:HIS:HE1	1:D:146:SER:OG	1.88	0.55
1:E:170[B]:VAL:HG11	1:E:203:LEU:HD13	1.88	0.55
1:A:77[B]:VAL:HG22	1:A:110:VAL:HG22	1.88	0.55
1:F:137:HIS:HE1	1:F:146:SER:OG	1.89	0.55
1:B:294:ARG:HG2	1:B:299[B]:ARG:HD3	1.88	0.55
1:B:70[B]:VAL:HG12	1:B:222:ILE:HD11	1.87	0.55
1:A:128:ARG:NH2	1:F:107:ARG:HH12	2.08	0.52
1:F:70:VAL:HG12	1:F:222:ILE:HD11	1.90	0.52
1:B:300:ILE:HD11	4:B:2171:HOH:O	2.11	0.51
1:A:34:VAL:HG22	1:A:105:LEU:HD22	1.93	0.50
1:A:128:ARG:HH21	1:F:107:ARG:NH1	2.08	0.50
1:C:53:SER:HA	1:C:60:THR:O	2.12	0.50
1:F:141:VAL:HG11	1:F:300:ILE:HD11	1.94	0.50
1:D:180:THR:O	1:D:183:MET:HG3	2.12	0.50
4:A:2256:HOH:O	1:F:223:THR:HG21	2.12	0.49
1:B:103:ARG:NH2	4:B:2115:HOH:O	2.41	0.49
1:C:220:PHE:HE1	1:C:260:MET:CE	2.26	0.49
1:C:155:THR:HG22	4:D:2161:HOH:O	2.12	0.48
1:B:53:SER:HA	1:B:60:THR:O	2.13	0.48
1:C:179:GLU:HG3	4:C:2186:HOH:O	2.13	0.48
1:C:70:VAL:HG12	1:C:222:ILE:HD11	1.96	0.47
1:F:180:THR:HA	1:F:183:MET:HE2	1.97	0.47
1:E:53:SER:HA	1:E:60:THR:O	2.14	0.47
1:A:53:SER:HA	1:A:60:THR:O	2.14	0.47
1:F:53:SER:HA	1:F:60:THR:O	2.15	0.47
1:B:151:VAL:HG21	1:B:163:LEU:HD21	1.97	0.47
1:B:180[B]:THR:HA	1:B:183:MET:HE2	1.96	0.47
1:E:183:MET:HG2	1:F:131:ALA:O	2.14	0.47
1:A:276:SER:OG	1:F:216:ARG:NH2	2.48	0.46
1:D:53:SER:HA	1:D:60:THR:O	2.16	0.46
1:B:70[B]:VAL:HG12	1:B:222:ILE:CD1	2.46	0.45
1:F:151:VAL:HG21	1:F:163:LEU:HD21	1.99	0.45
1:E:127:VAL:HG21	1:E:245[A]:ILE:HG12	1.99	0.45
1:C:127:VAL:HG21	1:C:245[A]:ILE:HG12	2.00	0.44
1:F:229:GLY:HA2	1:F:265:LYS:HB3	1.97	0.44
1:B:103:ARG:O	1:B:103:ARG:NH1	2.51	0.44
1:E:183:MET:HG3	4:E:2211:HOH:O	2.18	0.44
1:D:223:THR:HG21	4:E:2242:HOH:O	2.18	0.43
1:D:176:GLU:OE2	1:D:216:ARG:HD2	2.18	0.43
1:A:151:VAL:HG21	1:A:163:LEU:HD21	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:179:GLU:O	1:F:131:ALA:HB3	2.19	0.43
1:B:180[A]:THR:HA	1:B:183:MET:HE2	2.00	0.43
1:B:189:ALA:HB1	1:C:129:PRO:HD2	2.01	0.42
1:A:179[B]:GLU:HG2	1:B:294:ARG:HD3	1.99	0.42
1:A:221:GLY:HA3	1:B:124:LEU:HD22	2.01	0.42
1:E:39:VAL:CG2	1:F:59:MET:HE2	2.50	0.42
1:D:188:ILE:HD12	1:D:203:LEU:HD11	2.01	0.41
1:C:220:PHE:HE1	1:C:260:MET:HE1	1.85	0.41
1:D:151:VAL:HG21	1:D:163:LEU:HD21	2.02	0.41
1:F:142:ARG:HG2	4:F:2144:HOH:O	2.21	0.41
1:E:294:ARG:HG2	1:E:299:ARG:HD3	2.02	0.41
1:E:197[A]:LEU:HD21	1:E:242:LEU:HD22	2.01	0.41
1:C:77[B]:VAL:HG11	1:C:249:LEU:HD11	2.03	0.41
1:E:283:VAL:O	1:E:284:ASN:ND2	2.49	0.41
1:D:299:ARG:HH12	1:D:304:GLU:CD	2.30	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	272/358 (76%)	269 (99%)	3 (1%)	0	100	100
1	B	280/358 (78%)	276 (99%)	4 (1%)	0	100	100
1	C	275/358 (77%)	272 (99%)	3 (1%)	0	100	100
1	D	273/358 (76%)	268 (98%)	5 (2%)	0	100	100
1	E	277/358 (77%)	274 (99%)	3 (1%)	0	100	100
1	F	277/358 (77%)	274 (99%)	3 (1%)	0	100	100
All	All	1654/2148 (77%)	1633 (99%)	21 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	217/287 (76%)	214 (99%)	3 (1%)	59	46
1	B	223/287 (78%)	222 (100%)	1 (0%)	84	80
1	C	218/287 (76%)	213 (98%)	5 (2%)	44	27
1	D	215/287 (75%)	213 (99%)	2 (1%)	70	62
1	E	220/287 (77%)	219 (100%)	1 (0%)	81	76
1	F	219/287 (76%)	217 (99%)	2 (1%)	70	62
All	All	1312/1722 (76%)	1298 (99%)	14 (1%)	68	54

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	LYS
1	A	134	SER
1	A	299	ARG
1	B	134	SER
1	C	39	VAL
1	C	51	LYS
1	C	134	SER
1	C	299[A]	ARG
1	C	299[B]	ARG
1	D	134	SER
1	D	183	MET
1	E	134	SER
1	F	51	LYS
1	F	134	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	116	ASN
1	A	137	HIS
1	A	140	GLN

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Mol	Chain	Res	Type
1	A	291	GLN
1	B	137	HIS
1	B	140	GLN
1	B	291	GLN
1	C	137	HIS
1	C	140	GLN
1	C	284	ASN
1	C	291	GLN
1	D	116	ASN
1	D	137	HIS
1	D	140	GLN
1	D	291	GLN
1	E	116	ASN
1	E	137	HIS
1	E	140	GLN
1	E	291	GLN
1	F	137	HIS
1	F	140	GLN
1	F	291	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

6 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	GOL	E	1305	-	5,5,5	0.04	0	5,5,5	0.21	0
2	FLC	F	1307	-	12,12,12	1.11	0	17,17,17	1.19	1 (5%)
2	FLC	A	1304	-	12,12,12	1.04	0	17,17,17	1.20	1 (5%)
3	GOL	C	1304	-	5,5,5	0.25	0	5,5,5	0.18	0
3	GOL	D	1307	-	5,5,5	0.13	0	5,5,5	0.21	0
3	GOL	B	1304	-	5,5,5	0.14	0	5,5,5	0.36	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	E	1305	-	-	0/4/4/4	-
2	FLC	F	1307	-	-	2/16/16/16	-
2	FLC	A	1304	-	-	0/16/16/16	-
3	GOL	C	1304	-	-	0/4/4/4	-
3	GOL	D	1307	-	-	0/4/4/4	-
3	GOL	B	1304	-	-	0/4/4/4	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1304	FLC	OB1-CBC-CB	-2.41	117.42	122.09
2	F	1307	FLC	OB1-CBC-CB	-2.26	117.72	122.09

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	F	1307	FLC	CB-CA-CAC-OA2
2	F	1307	FLC	CB-CA-CAC-OA1

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2			OWAB(Å ²)	Q < 0.9
1	A	271/358 (75%)	-0.36	8 (2%)	52	56	7, 20, 43, 73	8 (2%)
1	B	270/358 (75%)	-0.38	9 (3%)	49	53	6, 16, 40, 69	16 (5%)
1	C	270/358 (75%)	-0.37	3 (1%)	78	81	6, 17, 40, 73	12 (4%)
1	D	273/358 (76%)	-0.47	2 (0%)	84	86	5, 15, 36, 65	5 (1%)
1	E	271/358 (75%)	-0.40	9 (3%)	49	53	5, 15, 37, 84	14 (5%)
1	F	272/358 (75%)	-0.40	3 (1%)	78	81	7, 17, 35, 56	12 (4%)
All	All	1627/2148 (75%)	-0.40	34 (2%)	63	68	5, 17, 39, 84	67 (4%)

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	303	GLY	5.2
1	A	303	GLY	4.3
1	D	228	PRO	4.3
1	F	306	ALA	3.9
1	B	228	PRO	3.8
1	B	34	VAL	3.7
1	D	306	ALA	3.5
1	B	303	GLY	3.2
1	B	301	PHE	3.2
1	F	228	PRO	3.1
1	F	35	ALA	3.0
1	E	181	PHE	2.7
1	B	229	GLY	2.6
1	A	301	PHE	2.6
1	B	133	LEU	2.6
1	E	34	VAL	2.6
1	E	92	SER	2.5
1	A	95	PRO	2.5
1	E	35	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	E	285	ASN	2.5
1	A	183	MET	2.5
1	E	223	THR	2.4
1	A	32	PRO	2.4
1	A	133	LEU	2.4
1	C	301	PHE	2.4
1	B	100	VAL	2.3
1	A	92	SER	2.3
1	E	183	MET	2.3
1	E	304	GLU	2.2
1	B	155	THR	2.1
1	C	155	THR	2.1
1	E	155	THR	2.1
1	A	35	ALA	2.1
1	B	35	ALA	2.1

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
2	FLC	A	1304	13/13	0.78	0.11	30,49,54,57	0
2	FLC	F	1307	13/13	0.88	0.08	24,34,37,39	0
3	GOL	D	1307	6/6	0.92	0.14	15,23,28,29	0
3	GOL	C	1304	6/6	0.93	0.14	16,28,32,35	0
3	GOL	B	1304	6/6	0.94	0.10	16,29,31,32	0
3	GOL	E	1305	6/6	0.96	0.08	13,27,33,35	0

6.5 Other polymers [i](#)

There are no such residues in this entry.