



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 08:39 AM UTC

PDB ID : 3BEW / pdb_00003bew
Title : 10mer Crystal Structure of chicken MHC class I haplotype B21
Authors : Koch, M.; Camp, S.; Collen, T.; Avila, D.; Salomonsen, J.; Wallny, H.J.; van Hateren, A.; Hunt, L.; Jacob, J.P.; Johnston, F.; Marston, D.A.; Shaw, I.; Dunbar, P.R.; Cerundolo, V.; Jones, E.Y.; Kaufman, J.
Deposited on : 2007-11-20
Resolution : 2.60 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
Xtrriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

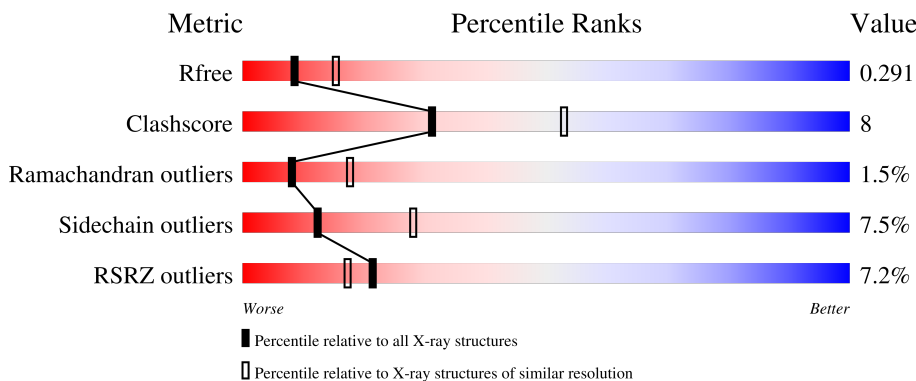
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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.



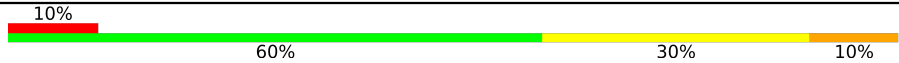
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	271	 6% 79% 18%
1	D	271	 12% 79% 19%
2	B	99	 4% 85% 14%
2	E	99	 3% 81% 17%
3	C	10	 80% 10% 10%

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Mol	Chain	Length	Quality of chain
3	F	10	 <p>A horizontal bar chart representing the quality of chain. The bar is divided into four segments: a red segment on the far left labeled '10%', a green segment labeled '60%', a yellow segment labeled '30%', and an orange segment on the far right labeled '10%'.</p>

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 6232 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 Major histocompatibility complex class I glycoprotein haplotype B21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	271	2182	1368	395	411	8	0	0	0
1	D	271	2182	1368	395	411	8	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	271	ARG	-	expression tag	UNP Q95601
D	271	ARG	-	expression tag	UNP Q95601

- Molecule 2 is a protein called Beta-2-microglobulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	99	787	504	127	150	6	0	0	0
2	E	99	787	504	127	150	6	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	0	MET	-	initiating methionine	UNP P21611
E	0	MET	-	initiating methionine	UNP P21611

- Molecule 3 is a protein called 10-mer from Tubulin beta-6 chain.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	C	10	83	50	14	19	0	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	F	10	Total	C	N	O	0	0	0
			83	50	14	19			

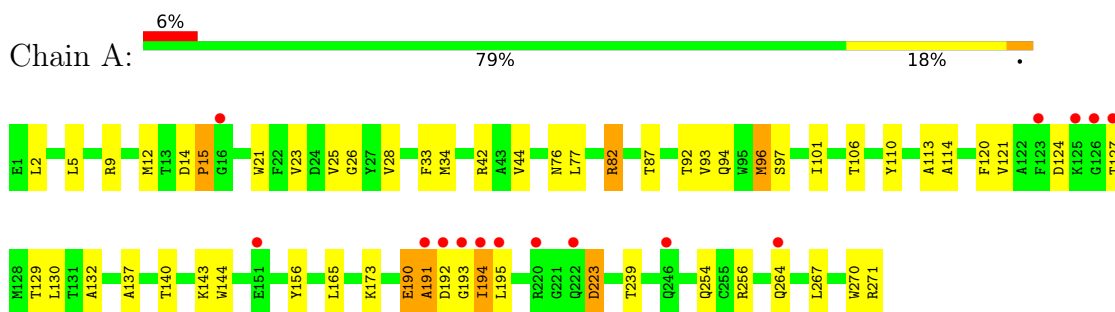
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	52	Total	O	0	0
			52	52		
4	B	35	Total	O	0	0
			35	35		
4	D	17	Total	O	0	0
			17	17		
4	E	23	Total	O	0	0
			23	23		
4	F	1	Total	O	0	0
			1	1		

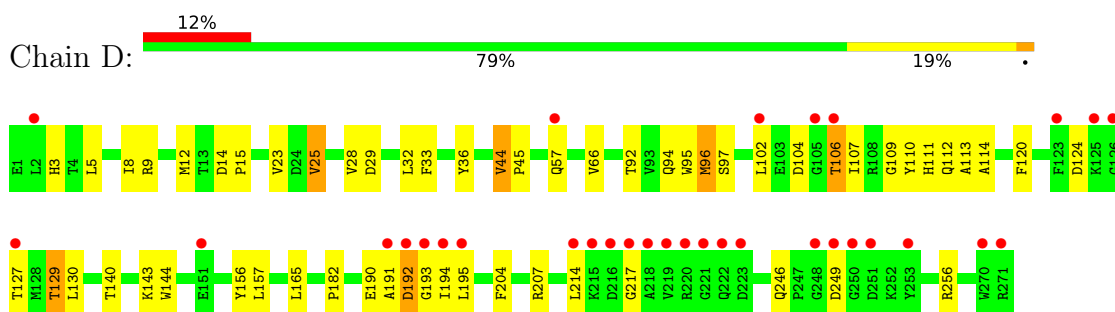
3 Residue-property plots [i](#)

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.

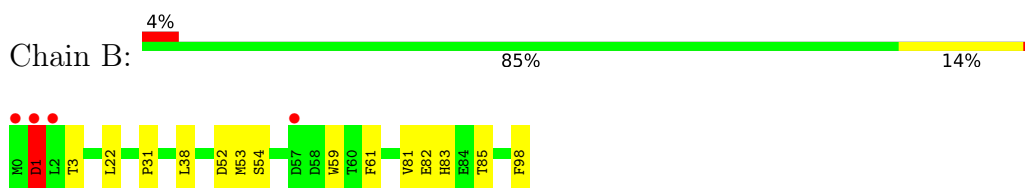
- Molecule 1: Major histocompatibility complex class I glycoprotein haplotype B21



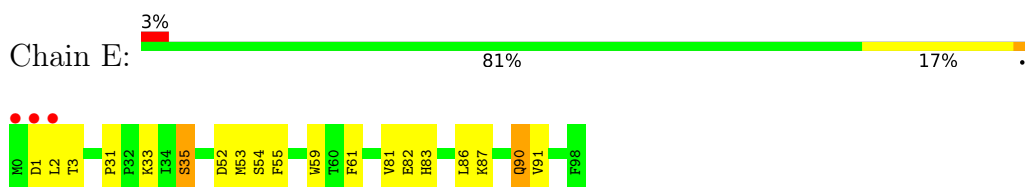
- Molecule 1: Major histocompatibility complex class I glycoprotein haplotype B21




- Molecule 2: Beta-2-microglobulin

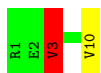


- Molecule 2: Beta-2-microglobulin



- Molecule 3: 10-mer from Tubulin beta-6 chain

Chain C:  80% 10% 10%



- Molecule 3: 10-mer from Tubulin beta-6 chain

Chain F:  10% 60% 30% 10%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	57.39Å 88.71Å 100.23Å 90.00° 80.01° 90.00°	Depositor
Resolution (Å)	29.15 – 2.60 29.15 – 2.60	Depositor EDS
% Data completeness (in resolution range)	97.5 (29.15-2.60) 97.9 (29.15-2.60)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.68 (at 2.61Å)	Xtrriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.234 , 0.295 0.233 , 0.291	Depositor DCC
R_{free} test set	1514 reflections (4.37%)	wwPDB-VP
Wilson B-factor (Å ²)	32.5	Xtrriage
Anisotropy	0.689	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 26.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	6232	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.06% 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

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	0.74	0/2241	0.84	4/3044 (0.1%)
1	D	0.73	0/2241	0.83	3/3044 (0.1%)
2	B	0.85	1/812 (0.1%)	0.85	1/1102 (0.1%)
2	E	0.91	3/812 (0.4%)	0.89	2/1102 (0.2%)
3	C	0.88	0/82	1.10	1/108 (0.9%)
3	F	0.59	0/82	0.95	0/108
All	All	0.77	4/6270 (0.1%)	0.85	11/8508 (0.1%)

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
1	A	1	0

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	91	VAL	CA-CB	-6.45	1.46	1.54
2	E	91	VAL	C-O	-5.60	1.18	1.24
2	E	91	VAL	CA-C	-5.57	1.45	1.52
2	B	81	VAL	C-O	-5.31	1.18	1.24

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	14	ASP	CA-C-N	7.55	126.82	118.97
1	D	14	ASP	C-N-CA	7.55	126.82	118.97
1	A	15	PRO	N-CA-C	7.03	123.52	113.47
1	A	14	ASP	CA-C-N	6.88	126.13	118.97
1	A	14	ASP	C-N-CA	6.88	126.13	118.97
2	E	81	VAL	N-CA-C	6.45	116.91	107.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	3	VAL	CB-CA-C	-6.07	103.12	111.49
2	E	82	GLU	N-CA-C	5.94	117.97	108.41
1	A	271	ARG	N-CA-C	5.92	127.58	111.00
1	D	15	PRO	N-CA-C	5.92	121.93	113.47
2	B	81	VAL	N-CA-C	5.57	115.91	108.11

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	271	ARG	CA

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2182	0	2069	34	0
1	D	2182	0	2069	41	0
2	B	787	0	746	13	0
2	E	787	0	746	12	0
3	C	83	0	84	5	0
3	F	83	0	84	12	0
4	A	52	0	0	0	0
4	B	35	0	0	0	0
4	D	17	0	0	0	0
4	E	23	0	0	1	0
4	F	1	0	0	1	0
All	All	6232	0	5798	97	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 8.

All (97) 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:D:96:MET:HE2	1:D:97:SER:N	1.87	0.90
1:A:156:TYR:CG	3:C:3:VAL:HG13	2.11	0.85
2:B:83:HIS:HD2	2:B:85:THR:OG1	1.62	0.83
1:D:96:MET:HE2	1:D:97:SER:CA	2.09	0.83
1:D:12:MET:HE1	2:E:53:MET:HG2	1.62	0.82
1:A:96:MET:HE1	1:A:110:TYR:HB2	1.62	0.81
1:A:127:THR:HG23	1:A:129:THR:HG22	1.67	0.77
2:E:53:MET:HE3	2:E:54:SER:H	1.48	0.77
1:A:124:ASP:OD2	1:A:127:THR:HG22	1.92	0.68
2:E:53:MET:HE2	2:E:61:PHE:HD1	1.59	0.68
1:D:96:MET:HE2	1:D:97:SER:C	2.20	0.67
1:A:156:TYR:CD1	3:C:3:VAL:HG13	2.30	0.66
2:E:53:MET:HE2	2:E:61:PHE:CD1	2.30	0.66
1:D:44:VAL:HG22	1:D:45:PRO:HD2	1.76	0.66
1:A:127:THR:CG2	1:A:129:THR:HG22	2.26	0.64
2:B:53:MET:CE	2:B:61:PHE:HB3	2.27	0.63
1:D:96:MET:CE	1:D:97:SER:C	2.71	0.63
1:D:95:TRP:CD2	3:F:8:LEU:HD22	2.35	0.62
2:E:86:LEU:HD13	2:E:90:GLN:HG3	1.81	0.61
1:D:140:THR:HG21	3:F:10:VAL:HG23	1.82	0.61
1:A:96:MET:HE1	1:A:110:TYR:CB	2.32	0.59
1:A:82:ARG:CG	1:A:82:ARG:HH11	2.16	0.59
2:B:53:MET:HE2	2:B:61:PHE:HB3	1.83	0.58
1:A:114:ALA:HB2	2:B:59:TRP:CE2	2.39	0.57
2:B:53:MET:HE2	2:B:61:PHE:CD1	2.40	0.56
2:B:83:HIS:CD2	2:B:85:THR:OG1	2.52	0.56
1:A:120:PHE:CD2	1:A:121:VAL:HG13	2.40	0.56
1:D:106:THR:C	1:D:107:ILE:HD13	2.31	0.55
2:E:53:MET:HE3	2:E:54:SER:N	2.20	0.54
1:D:120:PHE:CE2	3:F:10:VAL:CG2	2.91	0.54
1:D:120:PHE:CE2	3:F:10:VAL:HG22	2.44	0.53
1:D:156:TYR:CD1	3:F:3:VAL:HG13	2.43	0.53
1:D:127:THR:HG23	1:D:129:THR:OG1	2.08	0.53
1:D:156:TYR:CG	3:F:3:VAL:HG13	2.43	0.53
1:A:254:GLN:OE1	1:A:267:LEU:HD22	2.08	0.52
1:A:77:LEU:HD23	1:A:93:VAL:HG23	1.90	0.52
1:A:82:ARG:HH11	1:A:82:ARG:HG2	1.74	0.52
1:D:109:GLY:HA3	1:D:157:LEU:HD13	1.92	0.52
1:A:194:ILE:HD13	1:A:270:TRP:CD1	2.45	0.52
1:A:76:ASN:OD1	3:C:10:VAL:HG22	2.10	0.51
1:A:194:ILE:HG21	1:A:270:TRP:CD1	2.46	0.51
2:B:53:MET:HE3	2:B:54:SER:H	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:10:VAL:O	4:F:11:HOH:O	2.19	0.50
1:D:95:TRP:CG	3:F:8:LEU:HD22	2.46	0.50
1:A:193:GLY:C	1:A:194:ILE:HG13	2.36	0.50
2:B:53:MET:HE1	2:B:61:PHE:HB3	1.94	0.50
1:A:96:MET:HE2	1:A:97:SER:N	2.27	0.50
2:B:98:PHE:OXT	2:B:98:PHE:CG	2.65	0.49
2:B:31:PRO:O	2:B:83:HIS:HE1	1.95	0.49
3:F:10:VAL:OXT	3:F:10:VAL:HG13	2.13	0.49
1:D:8:ILE:HG23	2:E:55:PHE:CE2	2.47	0.49
2:B:22:LEU:HD23	2:B:38:LEU:HD22	1.95	0.48
1:A:191:ALA:O	1:A:193:GLY:N	2.46	0.48
1:D:8:ILE:HG23	2:E:55:PHE:CZ	2.48	0.48
1:D:106:THR:O	1:D:107:ILE:HD13	2.14	0.48
2:B:1:ASP:OD1	2:B:1:ASP:N	2.42	0.48
2:E:35:SER:HA	4:E:106:HOH:O	2.13	0.47
1:D:5:LEU:HB2	1:D:165:LEU:HD13	1.97	0.46
1:D:96:MET:HE1	1:D:110:TYR:HB2	1.97	0.46
1:D:246:GLN:HB2	1:D:249:ASP:OD2	2.15	0.46
1:D:25:VAL:HG12	1:D:32:LEU:HD11	1.97	0.46
1:D:94:GLN:O	1:D:113:ALA:HA	2.16	0.46
1:A:156:TYR:CD2	3:C:3:VAL:HG13	2.49	0.46
1:A:5:LEU:HB2	1:A:165:LEU:HD13	1.98	0.46
1:D:114:ALA:HB2	2:E:59:TRP:CE2	2.50	0.45
1:A:96:MET:HE2	1:A:96:MET:C	2.41	0.45
1:D:182:PRO:HB3	1:D:204:PHE:HB3	1.99	0.45
1:D:12:MET:HB3	1:D:92:THR:HG22	1.98	0.45
1:D:191:ALA:O	1:D:192:ASP:HB3	2.17	0.45
1:A:96:MET:HE2	1:A:97:SER:CA	2.47	0.45
1:A:15:PRO:HG3	1:A:21:TRP:HA	1.99	0.45
1:D:3:HIS:HA	1:D:29:ASP:OD1	2.18	0.44
1:D:156:TYR:CZ	3:F:3:VAL:HG22	2.53	0.44
1:A:26:GLY:HA3	1:A:34:MET:HG3	2.00	0.43
1:A:94:GLN:O	1:A:113:ALA:HA	2.18	0.43
1:D:120:PHE:HE2	3:F:10:VAL:CG2	2.30	0.43
1:D:191:ALA:O	1:D:192:ASP:CB	2.66	0.43
1:A:121:VAL:HG12	1:A:137:ALA:HB1	1.99	0.43
1:D:156:TYR:HD2	1:D:157:LEU:HD23	1.83	0.43
1:A:132:ALA:HB1	1:A:137:ALA:HB3	2.00	0.42
1:D:214:LEU:HD11	1:D:256:ARG:HH11	1.85	0.42
1:A:140:THR:HG23	3:C:10:VAL:HA	2.01	0.41
1:D:156:TYR:CE2	3:F:3:VAL:HG22	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:124:ASP:HB3	1:A:127:THR:HG22	2.03	0.41
1:D:28:VAL:HG23	1:D:33:PHE:CD1	2.56	0.41
1:A:28:VAL:HG23	1:A:33:PHE:CD1	2.55	0.41
2:B:98:PHE:OXT	2:B:98:PHE:CD1	2.74	0.41
2:E:53:MET:HE3	2:E:53:MET:HA	2.03	0.41
1:A:12:MET:HB3	1:A:92:THR:HG22	2.01	0.41
1:D:96:MET:HE2	1:D:96:MET:C	2.42	0.41
1:D:97:SER:OG	1:D:111:HIS:ND1	2.50	0.41
1:A:130:LEU:HD22	1:A:144:TRP:CD2	2.55	0.41
1:D:130:LEU:HD22	1:D:144:TRP:CD1	2.56	0.41
1:D:124:ASP:CG	1:D:127:THR:HG22	2.46	0.40
2:E:31:PRO:O	2:E:83:HIS:HE1	2.04	0.40
1:A:124:ASP:HB3	1:A:127:THR:CG2	2.51	0.40
1:D:36:TYR:CG	1:D:66:VAL:HG11	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	269/271 (99%)	251 (93%)	13 (5%)	5 (2%)	6	13
1	D	269/271 (99%)	251 (93%)	14 (5%)	4 (2%)	8	18
2	B	97/99 (98%)	96 (99%)	0	1 (1%)	12	28
2	E	97/99 (98%)	96 (99%)	0	1 (1%)	12	28
3	C	8/10 (80%)	8 (100%)	0	0	100	100
3	F	8/10 (80%)	8 (100%)	0	0	100	100
All	All	748/760 (98%)	710 (95%)	27 (4%)	11 (2%)	8	18

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	191	ALA
1	A	192	ASP
1	A	223	ASP
1	D	104	ASP
1	D	192	ASP
1	A	194	ILE
2	E	1	ASP
2	B	1	ASP
1	D	217	GLY
1	A	190	GLU
1	D	193	GLY

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	223/223 (100%)	204 (92%)	19 (8%)	10	22
1	D	223/223 (100%)	208 (93%)	15 (7%)	15	33
2	B	87/87 (100%)	83 (95%)	4 (5%)	24	49
2	E	87/87 (100%)	80 (92%)	7 (8%)	11	25
3	C	10/10 (100%)	9 (90%)	1 (10%)	7	16
3	F	10/10 (100%)	8 (80%)	2 (20%)	1	2
All	All	640/640 (100%)	592 (92%)	48 (8%)	12	28

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	LEU
1	A	9	ARG
1	A	23	VAL
1	A	25	VAL
1	A	42	ARG
1	A	44	VAL
1	A	82	ARG
1	A	87	THR

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Mol	Chain	Res	Type
1	A	96	MET
1	A	101	ILE
1	A	106	THR
1	A	143	LYS
1	A	173	LYS
1	A	190	GLU
1	A	195	LEU
1	A	223	ASP
1	A	239	THR
1	A	256	ARG
1	A	264	GLN
2	B	1	ASP
2	B	3	THR
2	B	52	ASP
2	B	82	GLU
3	C	3	VAL
1	D	9	ARG
1	D	23	VAL
1	D	25	VAL
1	D	44	VAL
1	D	57	GLN
1	D	96	MET
1	D	102	LEU
1	D	106	THR
1	D	112	GLN
1	D	129	THR
1	D	143	LYS
1	D	190	GLU
1	D	194	ILE
1	D	195	LEU
1	D	207	ARG
2	E	2	LEU
2	E	3	THR
2	E	33	LYS
2	E	35	SER
2	E	52	ASP
2	E	87	LYS
2	E	90	GLN
3	F	3	VAL
3	F	9	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	83	HIS
1	D	57	GLN
1	D	246	GLN
2	E	83	HIS

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 [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	271/271 (100%)	0.33	15 (5%) 30 25	14, 30, 48, 79	0
1	D	271/271 (100%)	0.63	32 (11%) 9 7	22, 33, 64, 102	0
2	B	99/99 (100%)	0.26	4 (4%) 42 37	16, 27, 42, 72	0
2	E	99/99 (100%)	0.14	3 (3%) 52 47	20, 29, 44, 74	0
3	C	10/10 (100%)	-0.23	0 100 100	18, 26, 33, 38	0
3	F	10/10 (100%)	0.90	1 (10%) 12 9	36, 42, 51, 54	0
All	All	760/760 (100%)	0.40	55 (7%) 21 17	14, 30, 50, 102	0

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	193	GLY	11.4
2	B	0	MET	11.4
1	A	194	ILE	10.8
2	B	1	ASP	6.8
1	D	194	ILE	6.5
1	D	219	VAL	5.6
2	E	0	MET	5.1
1	D	191	ALA	5.1
1	D	192	ASP	5.1
1	A	193	GLY	4.9
1	A	191	ALA	4.7
1	A	125	LYS	4.4
1	D	270	TRP	4.2
1	A	151	GLU	4.1
1	A	126	GLY	4.1
1	D	220	ARG	4.0
2	E	1	ASP	3.9
1	A	192	ASP	3.7
2	B	2	LEU	3.5

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Mol	Chain	Res	Type	RSRZ
1	D	102	LEU	3.3
1	D	223	ASP	3.2
3	F	10	VAL	3.2
1	A	195	LEU	3.2
1	D	215	LYS	3.1
1	D	57	GLN	3.0
1	A	222	GLN	2.9
1	D	253	TYR	2.9
1	D	250	GLY	2.9
1	D	218	ALA	2.8
1	A	16	GLY	2.8
1	D	195	LEU	2.7
1	D	216	ASP	2.7
1	D	217	GLY	2.7
1	D	221	GLY	2.7
1	D	127	THR	2.6
1	D	126	GLY	2.5
1	A	264	GLN	2.5
1	D	249	ASP	2.4
2	B	57	ASP	2.4
1	D	125	LYS	2.3
2	E	2	LEU	2.3
1	D	106	THR	2.3
1	A	220	ARG	2.3
1	A	123	PHE	2.3
1	D	151	GLU	2.3
1	A	127	THR	2.2
1	D	248	GLY	2.2
1	D	2	LEU	2.2
1	D	251	ASP	2.2
1	D	123	PHE	2.2
1	D	222	GLN	2.1
1	D	214	LEU	2.1
1	D	271	ARG	2.0
1	A	246	GLN	2.0
1	D	105	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 [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.