Full wwPDB X-ray Structure Validation Report ⓘ

Oct 22, 2023 – 02:54 AM EDT

PDB ID	:	2ZOL
Title	:	Crystal structure of H-2Db in complex with the W513S variant of JHMV epitope S510
Authors	:	Theodossis, A.; Dunstone, M.A.; Rossjohn, J.
Deposited on	:	2008-05-22
Resolution	:	2.70 Å(reported)

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

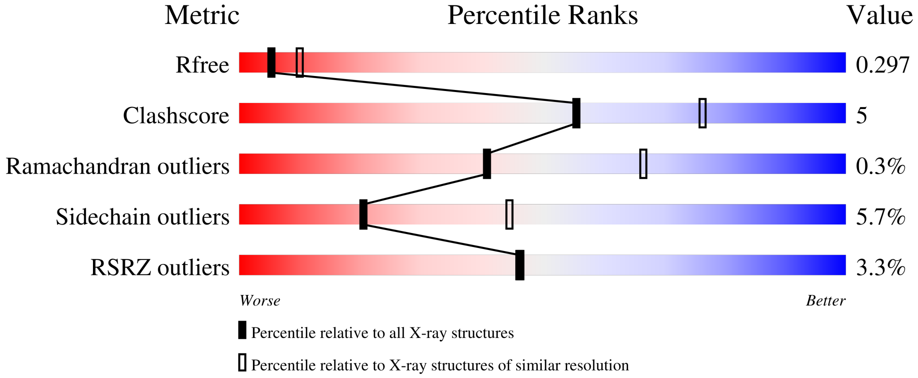
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance ⓘ

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

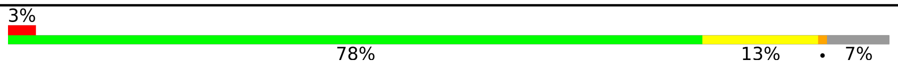
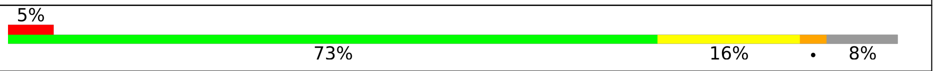
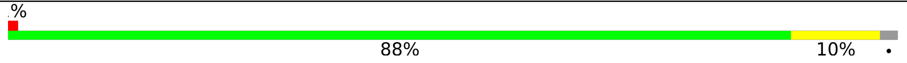
The reported resolution of this entry is 2.70 Å.

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}	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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 <=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	278	
1	C	278	
2	B	100	
2	D	100	
3	E	9	

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Mol	Chain	Length	Quality of chain
3	F	9	

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 6112 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 H-2 class I histocompatibility antigen, D-B alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	258	2126	1348	378	391	9	0	0	0
1	C	256	2111	1337	376	389	9	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	276	ARG	-	expression tag	UNP P01899
A	277	TRP	-	expression tag	UNP P01899
A	278	GLU	-	expression tag	UNP P01899
C	276	ARG	-	expression tag	UNP P01899
C	277	TRP	-	expression tag	UNP P01899
C	278	GLU	-	expression tag	UNP P01899

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	D	98	813	518	137	151	7	0	0	0
2	B	98	813	518	137	151	7	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	0	MET	-	initiating methionine	UNP P01887
B	0	MET	-	initiating methionine	UNP P01887

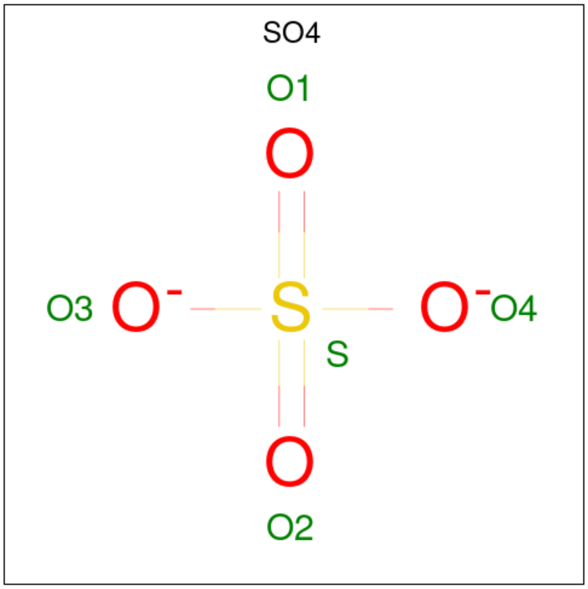
- Molecule 3 is a protein called 9-meric peptide from Spike glycoprotein.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
3	F	9	Total C N O 64 39 12 13	0	0	0
3	E	9	Total C N O 64 39 12 13	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	1	ABA	CYS	modified residue	UNP Q02385
F	4	SER	TRP	engineered mutation	UNP Q02385
E	1	ABA	CYS	modified residue	UNP Q02385
E	4	SER	TRP	engineered mutation	UNP Q02385

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	F	1	Total O S 5 4 1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	36	Total O 36 36	0	0
5	C	40	Total O 40 40	0	0

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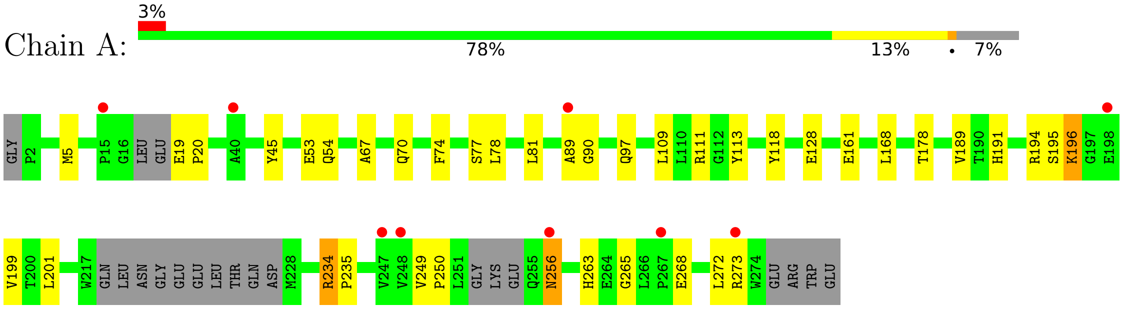
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	D	20	Total O 20 20	0	0
5	B	15	Total O 15 15	0	0
5	F	3	Total O 3 3	0	0
5	E	2	Total O 2 2	0	0

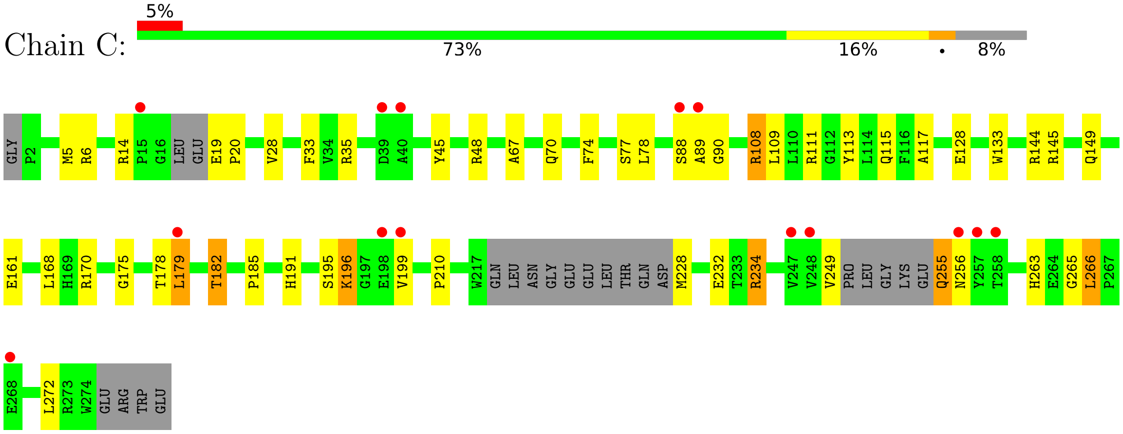
3 Residue-property plots ⓘ

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.

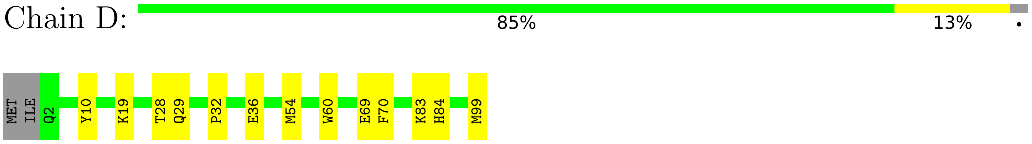
- Molecule 1: H-2 class I histocompatibility antigen, D-B alpha chain



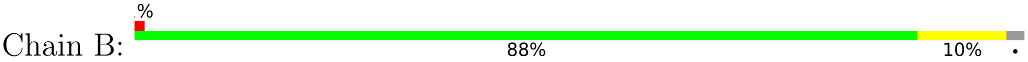
- Molecule 1: H-2 class I histocompatibility antigen, D-B alpha chain

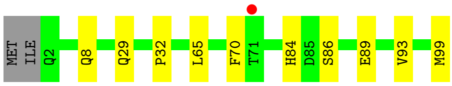


- Molecule 2: Beta-2-microglobulin



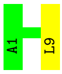
- Molecule 2: Beta-2-microglobulin





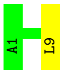
- Molecule 3: 9-meric peptide from Spike glycoprotein

Chain F:



- Molecule 3: 9-meric peptide from Spike glycoprotein

Chain E:



4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	83.56Å 71.03Å 87.00Å 90.00° 103.45° 90.00°	Depositor
Resolution (Å)	33.70 – 2.70 33.70 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.0 (33.70-2.70) 99.0 (33.70-2.70)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	3.05 (at 2.68Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.254 , 0.307 0.248 , 0.297	Depositor DCC
R_{free} test set	1368 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	36.6	Xtriage
Anisotropy	0.151	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 34.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	0.029 for l,-k,h	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	6112	wwPDB-VP
Average B, all atoms (Å^2)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.99% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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: SO4, ABA

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	0.31	0/2189	0.50	0/2969
1	C	0.32	0/2173	0.51	0/2946
2	B	0.34	0/839	0.51	0/1137
2	D	0.35	0/839	0.51	0/1137
3	E	0.24	0/59	0.59	0/78
3	F	0.24	0/59	0.53	0/78
All	All	0.32	0/6158	0.50	0/8345

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

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	2126	0	2006	26	0
1	C	2111	0	1988	28	0
2	B	813	0	782	6	0
2	D	813	0	782	7	0
3	E	64	0	63	1	0
3	F	64	0	63	1	0
4	F	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	36	0	0	0	0
5	B	15	0	0	0	0
5	C	40	0	0	0	0
5	D	20	0	0	0	0
5	E	2	0	0	0	0
5	F	3	0	0	0	0
All	All	6112	0	5684	59	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 5.

All (59) 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:35:ARG:NH2	2:D:54:MET:O	2.14	0.81
1:A:195:SER:O	1:A:196:LYS:HB2	1.91	0.70
1:C:195:SER:O	1:C:196:LYS:HB2	1.89	0.70
1:A:194:ARG:HG2	1:A:195:SER:H	1.57	0.70
1:A:234:ARG:HE	2:B:8:GLN:NE2	2.02	0.58
1:A:256:ASN:HA	1:A:273:ARG:HH21	1.69	0.58
1:A:189:VAL:HG11	1:A:273:ARG:O	2.05	0.57
1:A:249:VAL:HG12	1:A:250:PRO:O	2.05	0.56
1:A:191:HIS:CE1	1:A:199:VAL:HG11	2.40	0.56
1:C:185:PRO:HD2	1:C:266:LEU:HD13	1.90	0.54
1:A:77:SER:HB3	3:E:9:LEU:HD12	1.90	0.54
1:C:5:MET:HB2	1:C:168:LEU:HD13	1.91	0.52
1:C:263:HIS:CD2	1:C:265:GLY:H	2.27	0.52
2:D:36:GLU:HB2	2:D:83:LYS:HB3	1.91	0.52
1:A:109:LEU:HD22	1:A:161:GLU:HG2	1.93	0.51
1:A:263:HIS:CD2	1:A:265:GLY:H	2.28	0.51
1:A:45:TYR:CE2	1:A:67:ALA:HB2	2.47	0.49
1:C:111:ARG:HD3	1:C:113:TYR:CZ	2.47	0.48
1:C:234:ARG:HD3	2:D:10:TYR:CZ	2.48	0.48
1:C:117:ALA:HB2	2:D:60:TRP:CE2	2.48	0.48
1:A:256:ASN:N	1:A:256:ASN:ND2	2.61	0.48
1:C:249:VAL:HG11	1:C:255:GLN:HE21	1.78	0.48
2:D:32:PRO:O	2:D:84:HIS:HE1	1.97	0.48
1:C:175:GLY:O	1:C:179:LEU:HB2	2.14	0.48
1:C:109:LEU:HD22	1:C:161:GLU:HG2	1.96	0.47
2:B:32:PRO:O	2:B:84:HIS:HE1	1.97	0.47
1:C:133:TRP:HB2	1:C:144:ARG:HG3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:45:TYR:CE2	1:C:67:ALA:HB2	2.50	0.47
1:A:89:ALA:HA	1:A:90:GLY:HA2	1.67	0.47
1:A:234:ARG:NH2	2:B:99:MET:O	2.47	0.47
1:A:256:ASN:HA	1:A:273:ARG:NH2	2.29	0.47
1:C:195:SER:O	1:C:196:LYS:CB	2.59	0.46
1:A:234:ARG:HE	2:B:8:GLN:HE22	1.63	0.46
1:C:89:ALA:HA	1:C:90:GLY:HA2	1.69	0.46
1:C:108:ARG:HE	1:C:108:ARG:HB2	1.51	0.45
1:A:5:MET:HB2	1:A:168:LEU:HD13	1.98	0.45
2:D:28:THR:HG22	2:D:29:GLN:N	2.32	0.45
1:C:111:ARG:HG3	1:C:128:GLU:HG3	1.98	0.45
1:C:182:THR:HG21	1:C:265:GLY:HA2	1.99	0.45
1:A:45:TYR:HE2	1:A:67:ALA:HB2	1.81	0.45
1:A:70:GLN:O	1:A:74:PHE:HD1	2.01	0.44
1:C:28:VAL:HG23	1:C:33:PHE:CE1	2.52	0.44
1:A:195:SER:O	1:A:196:LYS:CB	2.63	0.43
1:C:185:PRO:HD2	1:C:266:LEU:CD1	2.48	0.43
1:A:201:LEU:HD12	1:A:249:VAL:HG21	2.00	0.43
1:C:19:GLU:HA	1:C:20:PRO:HD3	1.87	0.43
1:A:19:GLU:HA	1:A:20:PRO:HD3	1.90	0.41
1:C:263:HIS:HD2	1:C:265:GLY:H	1.67	0.41
1:A:111:ARG:HG3	1:A:128:GLU:HG3	2.02	0.41
1:C:70:GLN:O	1:C:74:PHE:HD1	2.04	0.41
1:C:77:SER:HB3	3:F:9:LEU:HD12	2.03	0.41
1:C:191:HIS:CE1	1:C:199:VAL:HG11	2.55	0.41
1:C:234:ARG:NH2	2:D:99:MET:O	2.53	0.41
1:A:81:LEU:HD13	1:A:118:TYR:CD1	2.56	0.41
1:C:133:TRP:O	1:C:144:ARG:NH1	2.54	0.41
2:B:84:HIS:CD2	2:B:86:SER:H	2.38	0.41
1:A:111:ARG:HD3	1:A:113:TYR:CZ	2.56	0.40
1:A:235:PRO:HG2	2:B:65:LEU:HD13	2.03	0.40
1:C:210:PRO:O	1:C:263:HIS:HE1	2.05	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	250/278 (90%)	243 (97%)	6 (2%)	1 (0%)	34	60
1	C	248/278 (89%)	241 (97%)	6 (2%)	1 (0%)	34	60
2	B	96/100 (96%)	94 (98%)	2 (2%)	0	100	100
2	D	96/100 (96%)	94 (98%)	2 (2%)	0	100	100
3	E	7/9 (78%)	7 (100%)	0	0	100	100
3	F	7/9 (78%)	7 (100%)	0	0	100	100
All	All	704/774 (91%)	686 (97%)	16 (2%)	2 (0%)	41	66

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	196	LYS
1	C	196	LYS

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	219/236 (93%)	210 (96%)	9 (4%)	30	59
1	C	217/236 (92%)	197 (91%)	20 (9%)	9	21
2	B	93/95 (98%)	89 (96%)	4 (4%)	29	57
2	D	93/95 (98%)	90 (97%)	3 (3%)	39	68
3	E	7/7 (100%)	7 (100%)	0	100	100
3	F	7/7 (100%)	7 (100%)	0	100	100
All	All	636/676 (94%)	600 (94%)	36 (6%)	20	44

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	53	GLU
1	A	54	GLN
1	A	78	LEU
1	A	97	GLN
1	A	178	THR
1	A	234	ARG
1	A	256	ASN
1	A	268	GLU
1	A	272	LEU
1	C	6	ARG
1	C	14	ARG
1	C	48	ARG
1	C	78	LEU
1	C	88	SER
1	C	108	ARG
1	C	115	GLN
1	C	145	ARG
1	C	149	GLN
1	C	170	ARG
1	C	178	THR
1	C	179	LEU
1	C	182	THR
1	C	228	MET
1	C	232	GLU
1	C	234	ARG
1	C	255	GLN
1	C	256	ASN
1	C	266	LEU
1	C	272	LEU
2	D	19	LYS
2	D	69	GLU
2	D	70	PHE
2	B	29	GLN
2	B	70	PHE
2	B	89	GLU
2	B	93	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	65	GLN
1	A	87	GLN
1	A	191	HIS

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Mol	Chain	Res	Type
1	A	192	HIS
1	A	256	ASN
1	A	263	HIS
1	C	72	GLN
1	C	87	GLN
1	C	255	GLN
1	C	263	HIS
2	D	8	GLN
2	D	17	ASN
2	D	38	GLN
2	D	84	HIS
2	B	8	GLN
2	B	84	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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	ABA	E	1	3	4,5,6	0.62	0	1,5,7	0.26	0
3	ABA	F	1	3	4,5,6	0.57	0	1,5,7	0.28	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	ABA	E	1	3	-	0/3/4/6	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ABA	F	1	3	-	0/3/4/6	-

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.

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

1 ligand is 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	$\#|Z| > 2$
4	SO4	F	10	-	4,4,4	0.16	0	6,6,6	0.16	0

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, 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	258/278 (92%)	0.20	9 (3%)	44	44	14, 27, 44, 48	10 (3%)
1	C	256/278 (92%)	0.25	14 (5%)	25	24	14, 27, 44, 48	9 (3%)
2	B	98/100 (98%)	-0.03	1 (1%)	82	83	14, 26, 34, 35	4 (4%)
2	D	98/100 (98%)	0.03	0	100	100	15, 26, 34, 36	1 (1%)
3	E	8/9 (88%)	0.18	0	100	100	14, 15, 16, 16	0
3	F	8/9 (88%)	0.38	0	100	100	14, 15, 15, 16	0
All	All	726/774 (93%)	0.17	24 (3%)	46	46	14, 26, 42, 48	24 (3%)

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	256	ASN	4.3
1	C	89	ALA	4.0
1	A	256	ASN	3.7
1	A	247	VAL	3.6
1	A	198	GLU	3.5
1	C	247	VAL	3.3
1	C	179	LEU	3.3
1	C	257	TYR	3.1
1	C	198	GLU	3.0
1	A	89	ALA	2.9
2	B	71	THR	2.7
1	C	40	ALA	2.7
1	A	40	ALA	2.6
1	C	268	GLU	2.6
1	C	258	THR	2.4
1	A	248	VAL	2.4
1	A	267	PRO	2.4
1	C	39	ASP	2.4
1	C	15	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	88	SER	2.2
1	A	15	PRO	2.1
1	C	199	VAL	2.0
1	A	273	ARG	2.0
1	C	248	VAL	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (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
3	ABA	F	1	6/7	0.97	0.13	13,13,14,14	0
3	ABA	E	1	6/7	0.97	0.14	13,13,14,14	0

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
4	SO4	F	10	5/5	0.97	0.17	25,25,26,26	0

6.5 Other polymers (i)

There are no such residues in this entry.