



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 09:15 PM UTC

PDB ID : 8PMW / pdb_00008pmw
Title : HEV gt3 P domain in complex with glycan-sensitive nAb p60.1
Authors : Ssebyatika, G.; Krey, T.
Deposited on : 2023-06-29
Resolution : 1.98 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

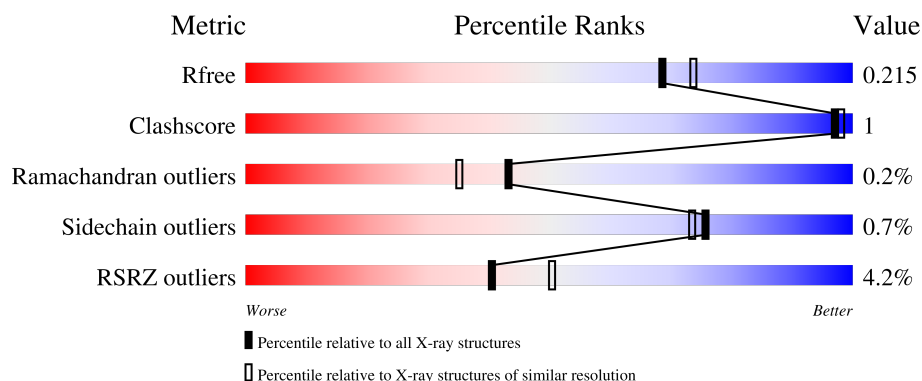
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.98 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	1506 (1.98-1.98)
Clashscore	190562	1534 (1.98-1.98)
Ramachandran outliers	187476	1518 (1.98-1.98)
Sidechain outliers	187428	1518 (1.98-1.98)
RSRZ outliers	180081	1506 (1.98-1.98)

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	251	0% 41% 57%
1	B	251	5% 43% 5% 52%
1	G	251	3% 43% 53%
1	H	251	2% 41% 57%
2	C	211	2% 73% 26%

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Mol	Chain	Length	Quality of chain
2	D	211	2% 72% 27%
2	E	211	2% 70% 28%
2	F	211	2% 74% 26%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8498 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 scFv_p60.1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	107	Total	C	N	O	S	0	0	0
			803	501	138	161	3			
1	B	120	Total	C	N	O	S	0	0	0
			948	601	164	181	2			
1	G	119	Total	C	N	O	S	0	0	0
			942	598	163	179	2			
1	H	107	Total	C	N	O	S	0	0	0
			803	501	138	161	3			

- Molecule 2 is a protein called Capsid protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	156	Total	C	N	O	S	0	0	0
			1179	750	197	231	1			
2	D	153	Total	C	N	O	S	0	0	0
			1162	737	194	230	1			
2	E	151	Total	C	N	O	S	0	0	0
			1148	730	192	225	1			
2	F	156	Total	C	N	O	S	0	0	0
			1179	750	197	231	1			

There are 28 discrepancies between the modelled and reference sequences:

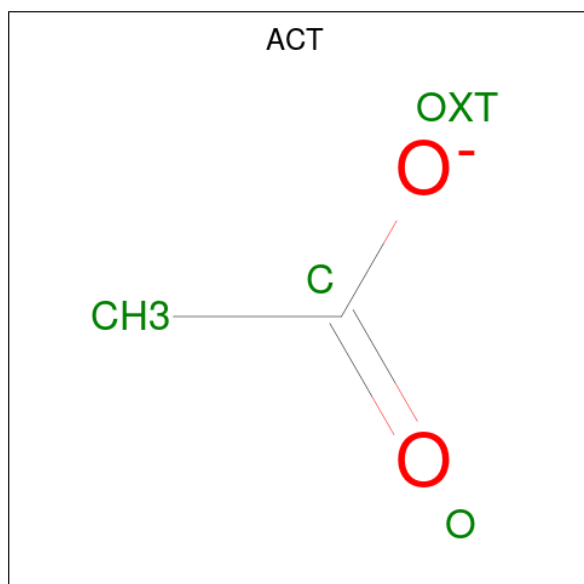
Chain	Residue	Modelled	Actual	Comment	Reference
C	463	GLY	-	expression tag	UNP A0A6C0PR31
C	464	ASP	-	expression tag	UNP A0A6C0PR31
C	465	ASP	-	expression tag	UNP A0A6C0PR31
C	466	ASP	-	expression tag	UNP A0A6C0PR31
C	467	ASP	-	expression tag	UNP A0A6C0PR31
C	468	LYS	-	expression tag	UNP A0A6C0PR31
C	513	PHE	LEU	conflict	UNP A0A6C0PR31
D	463	GLY	-	expression tag	UNP A0A6C0PR31

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Chain	Residue	Modelled	Actual	Comment	Reference
D	464	ASP	-	expression tag	UNP A0A6C0PR31
D	465	ASP	-	expression tag	UNP A0A6C0PR31
D	466	ASP	-	expression tag	UNP A0A6C0PR31
D	467	ASP	-	expression tag	UNP A0A6C0PR31
D	468	LYS	-	expression tag	UNP A0A6C0PR31
D	513	PHE	LEU	conflict	UNP A0A6C0PR31
E	463	GLY	-	expression tag	UNP A0A6C0PR31
E	464	ASP	-	expression tag	UNP A0A6C0PR31
E	465	ASP	-	expression tag	UNP A0A6C0PR31
E	466	ASP	-	expression tag	UNP A0A6C0PR31
E	467	ASP	-	expression tag	UNP A0A6C0PR31
E	468	LYS	-	expression tag	UNP A0A6C0PR31
E	513	PHE	LEU	conflict	UNP A0A6C0PR31
F	463	GLY	-	expression tag	UNP A0A6C0PR31
F	464	ASP	-	expression tag	UNP A0A6C0PR31
F	465	ASP	-	expression tag	UNP A0A6C0PR31
F	466	ASP	-	expression tag	UNP A0A6C0PR31
F	467	ASP	-	expression tag	UNP A0A6C0PR31
F	468	LYS	-	expression tag	UNP A0A6C0PR31
F	513	PHE	LEU	conflict	UNP A0A6C0PR31

- Molecule 3 is ACETATE ION (CCD ID: ACT) (formula: C₂H₃O₂).



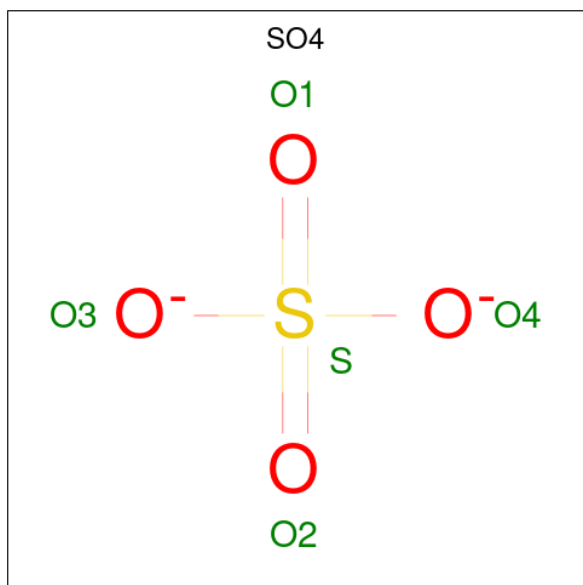
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	C	1	Total	C	O	0	0
			4	2	2		
3	D	1	Total	C	O	0	0
			4	2	2		
3	G	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

- Molecule 5 is water.

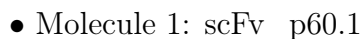
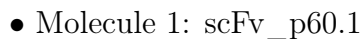
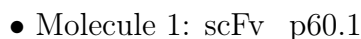
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	24	Total	O	0	0
			24	24		
5	B	23	Total	O	0	0
			23	23		
5	C	47	Total	O	0	0
			47	47		
5	D	76	Total	O	0	0
			76	76		

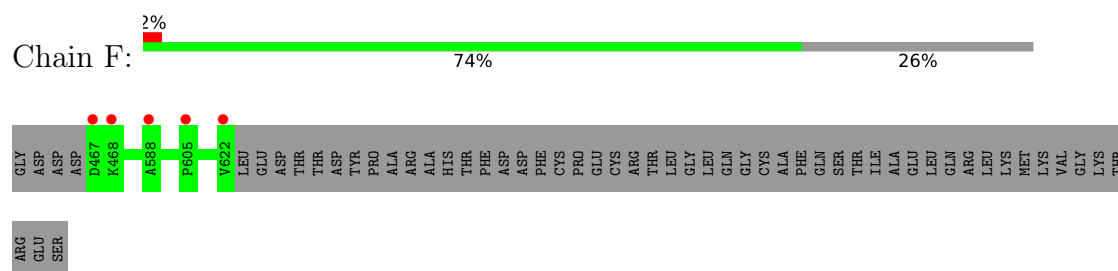
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	E	71	Total 71	O 71	0	0
5	F	40	Total 40	O 40	0	0
5	G	8	Total 8	O 8	0	0
5	H	19	Total 19	O 19	0	0

- Molecule 1: scFv p60.1





4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	75.81Å 159.26Å 205.67Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.44 – 1.98 48.44 – 1.98	Depositor EDS
% Data completeness (in resolution range)	99.5 (48.44-1.98) 99.5 (48.44-1.98)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.38 (at 1.98Å)	Xtriage
Refinement program	BUSTER 2.10.4	Depositor
R, R_{free}	0.206 , 0.227 0.195 , 0.215	Depositor DCC
R_{free} test set	4316 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	42.2	Xtriage
Anisotropy	0.227	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 33.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	8498	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.38% 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

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, ACT

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	0.69	0/822	0.93	1/1117 (0.1%)
1	B	0.65	0/974	0.89	2/1330 (0.2%)
1	G	0.68	0/968	0.91	0/1322
1	H	0.71	0/822	0.94	0/1117
2	C	0.62	0/1208	0.93	1/1658 (0.1%)
2	D	0.71	0/1191	0.93	0/1634
2	E	0.67	0/1177	0.92	1/1615 (0.1%)
2	F	0.66	0/1208	0.92	0/1658
All	All	0.67	0/8370	0.92	5/11451 (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	A	26	ASN	CA-CB-CG	6.77	119.37	112.60
1	B	106	THR	N-CA-C	-5.19	102.02	109.24
2	C	515	ASN	N-CA-C	-5.08	100.80	108.67
1	B	109	ASP	CA-CB-CG	5.04	117.64	112.60
2	E	515	ASN	N-CA-C	-5.02	100.89	108.67

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	803	0	770	2	0
1	B	948	0	917	6	0
1	G	942	0	912	7	0
1	H	803	0	770	2	0
2	C	1179	0	1161	0	0
2	D	1162	0	1135	0	0
2	E	1148	0	1126	1	0
2	F	1179	0	1161	0	0
3	A	4	0	3	0	0
3	C	4	0	3	0	0
3	D	4	0	3	0	0
3	G	4	0	3	0	0
4	A	5	0	0	0	0
4	H	5	0	0	0	0
5	A	24	0	0	0	0
5	B	23	0	0	0	0
5	C	47	0	0	0	0
5	D	76	0	0	0	0
5	E	71	0	0	0	0
5	F	40	0	0	0	0
5	G	8	0	0	0	0
5	H	19	0	0	0	0
All	All	8498	0	7964	15	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 1.

All (15) 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:G:40:ARG:NH2	1:G:45:ARG:HH12	1.82	0.78
1:B:69:GLY:HA2	1:G:69:GLY:HA3	1.74	0.70
1:G:40:ARG:NH2	1:G:45:ARG:NH1	2.49	0.60
1:G:107:PRO:HG3	1:H:34:ASN:CG	2.32	0.54
1:A:34:ASN:CG	1:B:107:PRO:HG3	2.36	0.50
1:G:40:ARG:HH21	1:G:45:ARG:NH1	2.14	0.45
1:B:18:LEU:HD12	1:B:117:VAL:HG11	1.99	0.43
1:B:101:ARG:O	1:B:108:PHE:HA	2.19	0.43
1:A:37:GLN:HB2	1:A:47:LEU:HD11	2.01	0.43
2:E:511:VAL:HG21	2:E:592:VAL:HB	2.01	0.43
1:G:101:ARG:O	1:G:108:PHE:HA	2.19	0.42
1:B:14:PRO:HD3	1:B:120:SER:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:35:ALA:HA	1:B:54:TYR:HB3	2.03	0.41
1:G:35:ALA:HA	1:G:54:TYR:HB3	2.02	0.41
1:H:37:GLN:HB2	1:H:47:LEU:HD11	2.03	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	105/251 (42%)	101 (96%)	4 (4%)	0	100	100
1	B	118/251 (47%)	113 (96%)	4 (3%)	1 (1%)	16	7
1	G	117/251 (47%)	111 (95%)	5 (4%)	1 (1%)	14	6
1	H	105/251 (42%)	102 (97%)	3 (3%)	0	100	100
2	C	154/211 (73%)	150 (97%)	4 (3%)	0	100	100
2	D	151/211 (72%)	146 (97%)	5 (3%)	0	100	100
2	E	149/211 (71%)	145 (97%)	4 (3%)	0	100	100
2	F	154/211 (73%)	149 (97%)	5 (3%)	0	100	100
All	All	1053/1848 (57%)	1017 (97%)	34 (3%)	2 (0%)	43	35

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	107	PRO
1	G	107	PRO

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	91/206 (44%)	91 (100%)	0	100	100
1	B	105/206 (51%)	104 (99%)	1 (1%)	68	65
1	G	104/206 (50%)	102 (98%)	2 (2%)	50	44
1	H	91/206 (44%)	89 (98%)	2 (2%)	45	38
2	C	127/174 (73%)	127 (100%)	0	100	100
2	D	126/174 (72%)	125 (99%)	1 (1%)	73	71
2	E	124/174 (71%)	124 (100%)	0	100	100
2	F	127/174 (73%)	127 (100%)	0	100	100
All	All	895/1520 (59%)	889 (99%)	6 (1%)	76	73

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	102	ASP
2	D	468	LYS
1	G	58	LYS
1	G	102	ASP
1	H	1	ASP
1	H	11	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	GLN
1	A	26	ASN
1	B	16	GLN
2	C	495	GLN
2	C	573	ASN
2	D	495	GLN
2	E	495	GLN
2	F	495	GLN

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Mol	Chain	Res	Type
1	G	3	GLN
1	H	3	GLN
1	H	79	GLN

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](#)

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	$\# Z > 2$
4	SO4	H	201	-	4,4,4	0.44	0	6,6,6	0.29	0
3	ACT	D	701	-	3,3,3	1.16	0	3,3,3	1.52	1 (33%)
4	SO4	A	202	-	4,4,4	0.24	0	6,6,6	0.21	0
3	ACT	A	201	-	3,3,3	0.95	0	3,3,3	1.33	0
3	ACT	C	701	-	3,3,3	0.91	0	3,3,3	1.57	1 (33%)
3	ACT	G	301	-	3,3,3	0.63	0	3,3,3	1.97	2 (66%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	301	ACT	O-C-CH3	-2.48	112.37	122.53
3	G	301	ACT	OXT-C-O	2.31	130.58	122.03
3	D	701	ACT	OXT-C-O	2.07	129.72	122.03
3	C	701	ACT	OXT-C-O	2.02	129.50	122.03

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 [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	107/251 (42%)	0.30	2 (1%) 66 75	35, 44, 58, 67	0
1	B	120/251 (47%)	0.80	13 (10%) 11 15	35, 49, 86, 98	0
1	G	119/251 (47%)	0.57	7 (5%) 28 37	34, 44, 76, 93	0
1	H	107/251 (42%)	0.31	6 (5%) 30 38	33, 44, 57, 70	0
2	C	156/211 (73%)	0.36	4 (2%) 57 67	35, 46, 62, 73	0
2	D	153/211 (72%)	0.11	4 (2%) 57 67	32, 39, 50, 82	0
2	E	151/211 (71%)	0.15	4 (2%) 57 67	30, 39, 50, 68	0
2	F	156/211 (73%)	0.53	5 (3%) 50 60	35, 46, 61, 69	0
All	All	1069/1848 (57%)	0.38	45 (4%) 40 50	30, 44, 66, 98	0

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	622	VAL	7.2
2	C	622	VAL	5.2
1	G	12	VAL	5.0
1	G	11	LEU	4.2
1	B	11	LEU	3.5
1	B	12	VAL	3.5
1	G	14	PRO	3.4
1	G	15	SER	3.4
2	C	467	ASP	3.4
2	D	467	ASP	3.2
1	B	120	SER	3.1
2	E	467	ASP	3.0
2	E	617	HIS	3.0
1	G	9	PRO	2.9
1	B	9	PRO	2.8
1	H	107	LYS	2.8

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Mol	Chain	Res	Type	RSRZ
2	F	467	ASP	2.7
2	D	466	ASP	2.7
2	F	588	ALA	2.6
1	B	66	SER	2.6
1	B	67	VAL	2.5
1	G	119	VAL	2.5
1	B	119	VAL	2.5
1	H	7	SER	2.4
1	H	9	SER	2.4
2	D	618	SER	2.4
1	A	107	LYS	2.4
1	B	18	LEU	2.4
1	H	5	THR	2.4
2	D	537	ARG	2.4
1	A	1	ASP	2.3
1	H	1	ASP	2.3
2	F	605	PRO	2.2
2	E	564	GLY	2.2
2	C	543	GLN	2.2
1	B	15	SER	2.2
1	B	43	PRO	2.2
2	E	537	ARG	2.2
1	G	1	GLU	2.1
1	B	26	GLY	2.1
1	B	79	LYS	2.1
1	H	26	ASN	2.1
2	C	468	LYS	2.1
2	F	468	LYS	2.0
1	B	10	GLY	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](#)

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(Å ²)	Q<0.9
3	ACT	C	701	4/4	0.38	0.28	66,66,66,67	0
3	ACT	D	701	4/4	0.51	0.29	67,68,68,68	0
3	ACT	G	301	4/4	0.62	0.24	68,68,68,68	0
3	ACT	A	201	4/4	0.83	0.21	54,54,54,54	0
4	SO4	H	201	5/5	0.94	0.09	56,57,57,57	0
4	SO4	A	202	5/5	0.95	0.08	50,51,52,52	0

6.5 Other polymers [i](#)

There are no such residues in this entry.