



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 20, 2020 – 01:13 PM BST

PDB ID : 5KR5
Title : Directed Evolution of Transaminases By Ancestral Reconstruction. Using Old Proteins for New Chemistries
Authors : Wilding, M.; Newman, J.; Peat, T.S.; Scott, C.
Deposited on : 2016-07-07
Resolution : 2.10 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 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 : 2.13.1
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) : 2.13.1

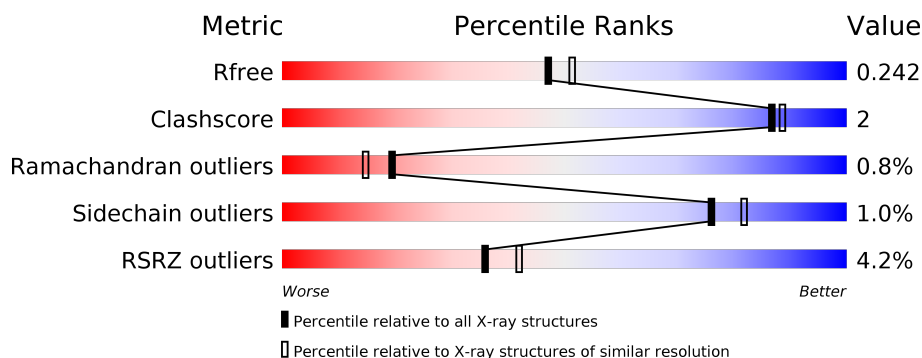
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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 on 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	479	<div> <div>4%</div> <div> <div></div> <div>88%</div> <div>7%</div> <div>5%</div> </div> </div>
1	B	479	<div> <div>4%</div> <div> <div></div> <div>87%</div> <div>7%</div> <div>5%</div> </div> </div>

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 7403 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 4-aminobutyrate transaminase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	455	Total	C	N	O	S	0	3	0
			3503	2232	605	652	14			
1	B	454	Total	C	N	O	S	0	2	0
			3488	2219	603	652	14			

- Molecule 2 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula: $C_8H_{10}NO_6P$).

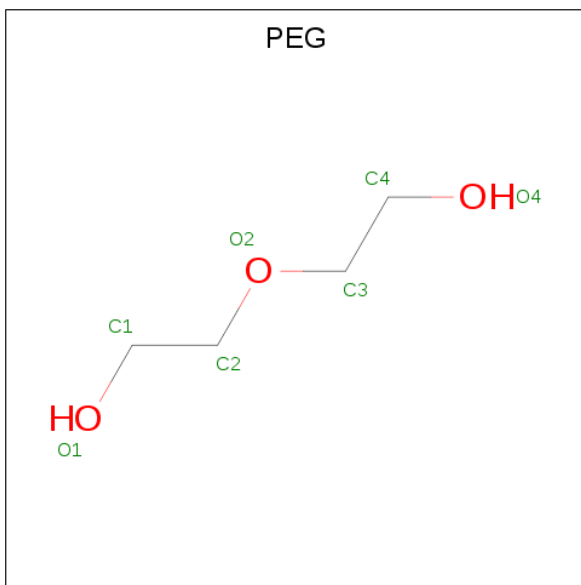


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	B	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total Ca 1 1	0	0
3	A	2	Total Ca 2 2	0	0

- Molecule 4 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C₄H₁₀O₃).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 7 4 3	0	0
4	A	1	Total C O 7 4 3	0	0
4	B	1	Total C O 7 4 3	0	0

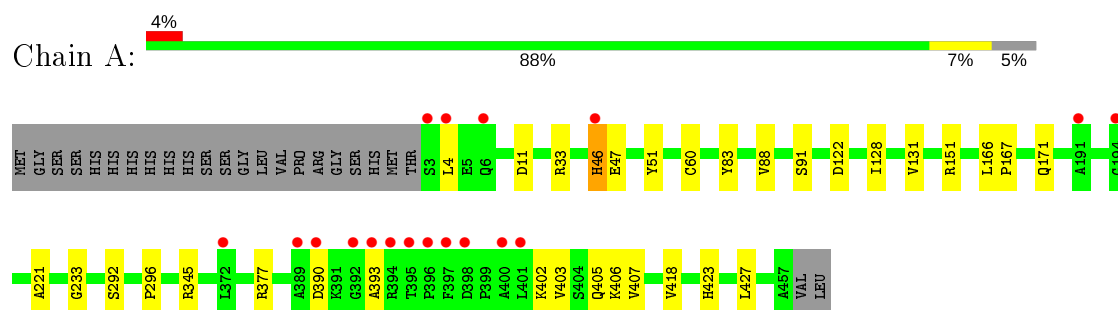
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	204	Total O 204 204	0	0
5	B	154	Total O 154 154	0	0

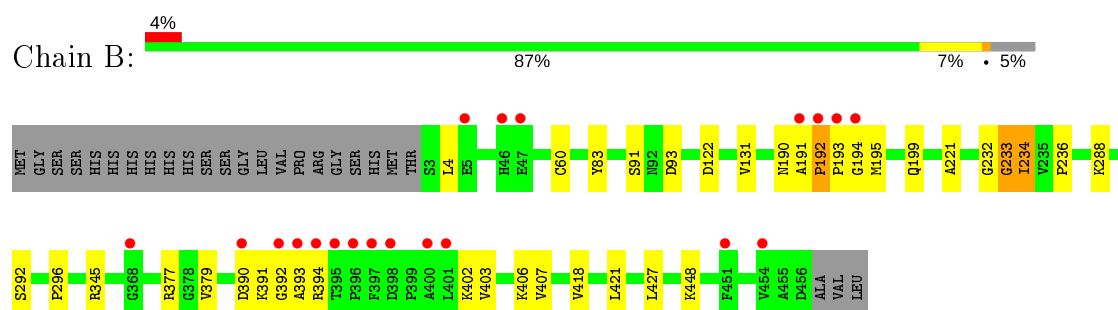
3 Residue-property plots [i](#)

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: 4-aminobutyrate transaminase



- Molecule 1: 4-aminobutyrate transaminase



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	98.45Å 102.54Å 199.78Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.60 – 2.10 47.80 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.4 (48.60-2.10) 99.4 (47.80-2.10)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.00 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.8.0155	Depositor
R, R_{free}	0.204 , 0.240 0.211 , 0.242	Depositor DCC
R_{free} test set	2892 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å ²)	24.0	Xtriage
Anisotropy	0.095	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 38.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.047 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	7403	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.33% 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: CA, PEG, PLP

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	0.48	0/3589	0.71	3/4878 (0.1%)
1	B	0.47	0/3574	0.70	4/4856 (0.1%)
All	All	0.48	0/7163	0.71	7/9734 (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	0	2
1	B	0	5
All	All	0	7

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	345	ARG	NE-CZ-NH1	5.49	123.04	120.30
1	B	288	LYS	CD-CE-NZ	5.43	124.18	111.70
1	B	122	ASP	CB-CG-OD1	5.33	123.10	118.30
1	A	377	ARG	NE-CZ-NH1	5.33	122.96	120.30
1	A	122	ASP	CB-CG-OD1	5.29	123.06	118.30
1	B	345	ARG	NE-CZ-NH1	5.18	122.89	120.30
1	B	377	ARG	NE-CZ-NH1	5.09	122.85	120.30

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	46	HIS	Peptide
1	A	83	TYR	Peptide
1	B	191	ALA	Peptide
1	B	192	PRO	Peptide
1	B	232	GLY	Peptide
1	B	391	LYS	Peptide
1	B	83	TYR	Peptide

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	3503	0	3436	16	0
1	B	3488	0	3413	14	0
2	A	15	0	6	0	0
2	B	15	0	6	0	0
3	A	2	0	0	0	0
3	B	1	0	0	0	0
4	A	14	0	20	0	0
4	B	7	0	10	0	0
5	A	204	0	0	1	0
5	B	154	0	0	0	0
All	All	7403	0	6891	29	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 2.

All (29) 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:A:11:ASP:OD2	5:A:601:HOH:O	2.17	0.59
1:A:4:LEU:HD13	1:A:46:HIS:ND1	2.18	0.58
1:A:131[A]:VAL:CG1	1:A:221:ALA:HB1	2.35	0.56
1:B:195:MET:HG2	1:B:199:GLN:HB3	1.87	0.56
1:B:236:PRO:HG3	1:B:379:VAL:HG23	1.87	0.56
1:A:4:LEU:HD13	1:A:46:HIS:CG	2.41	0.55
1:A:402:LYS:HB3	1:A:405:GLN:OE1	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:131:VAL:CG1	1:B:221:ALA:HB1	2.38	0.54
1:B:60:CYS:O	1:B:292:SER:HA	2.09	0.53
1:A:60:CYS:O	1:A:292:SER:HA	2.09	0.52
1:A:403:VAL:O	1:A:407:VAL:HG23	2.14	0.48
1:A:418:VAL:HG23	1:A:427:LEU:HD11	1.97	0.47
1:A:151:ARG:HD2	1:A:423:HIS:CE1	2.50	0.46
1:A:390:ASP:OD1	1:A:393:ALA:N	2.42	0.46
1:A:402:LYS:O	1:A:406:LYS:HG3	2.15	0.46
1:A:128:ILE:HA	1:A:131[B]:VAL:HG22	1.98	0.45
1:B:403:VAL:O	1:B:407:VAL:HG23	2.17	0.45
1:A:33:ARG:NH1	1:A:51:TYR:OH	2.50	0.44
1:A:88[B]:VAL:HG23	1:A:88[B]:VAL:O	2.19	0.43
1:A:166:LEU:HA	1:A:167:PRO:HD3	1.91	0.43
1:B:233:GLY:HA2	1:B:421:LEU:CD1	2.50	0.42
1:B:402:LYS:O	1:B:406:LYS:HG3	2.20	0.41
1:B:390:ASP:OD1	1:B:393:ALA:N	2.39	0.41
1:B:418:VAL:HG23	1:B:427:LEU:HD11	2.01	0.41
1:A:296:PRO:HG2	1:B:296:PRO:HG2	2.03	0.41
1:B:236:PRO:CG	1:B:379:VAL:HG23	2.50	0.40
1:B:4:LEU:O	1:B:4:LEU:HD12	2.21	0.40
1:B:192:PRO:HB2	1:B:195:MET:SD	2.61	0.40
1:B:234:ILE:HG12	1:B:421:LEU:HD11	2.03	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	456/479 (95%)	430 (94%)	24 (5%)	2 (0%)	34	32
1	B	454/479 (95%)	431 (95%)	18 (4%)	5 (1%)	14	9
All	All	910/958 (95%)	861 (95%)	42 (5%)	7 (1%)	19	15

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	47	GLU
1	B	392	GLY
1	B	194	GLY
1	B	233	GLY
1	A	233	GLY
1	B	193	PRO
1	B	234	ILE

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	357/375 (95%)	355 (99%)	2 (1%)	86	90
1	B	356/375 (95%)	351 (99%)	5 (1%)	67	73
All	All	713/750 (95%)	706 (99%)	7 (1%)	76	82

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	91	SER
1	A	171	GLN
1	B	91	SER
1	B	93	ASP
1	B	190	ASN
1	B	394	ARG
1	B	448	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	423	HIS
1	B	190	ASN
1	B	364	HIS

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 8 ligands modelled in this entry, 3 are monoatomic - leaving 5 for Mogul analysis.

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	PEG	B	503	-	6,6,6	0.39	0	5,5,5	0.53	0
2	PLP	B	501	1	15,15,16	3.61	3 (20%)	20,22,23	2.22	4 (20%)
2	PLP	A	501	1	15,15,16	3.28	3 (20%)	20,22,23	2.29	6 (30%)
4	PEG	A	504	-	6,6,6	0.37	0	5,5,5	0.38	0
4	PEG	A	505	-	6,6,6	0.36	0	5,5,5	0.43	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
4	PEG	B	503	-	-	1/4/4/4	-
2	PLP	B	501	1	-	0/6/6/8	0/1/1/1
2	PLP	A	501	1	-	0/6/6/8	0/1/1/1
4	PEG	A	504	-	-	3/4/4/4	-
4	PEG	A	505	-	-	1/4/4/4	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	PLP	C5-C4	10.91	1.52	1.40
2	A	501	PLP	C5-C4	9.24	1.50	1.40
2	A	501	PLP	C3-C2	7.31	1.48	1.40
2	B	501	PLP	C3-C2	7.14	1.48	1.40
2	B	501	PLP	C3-C4	4.18	1.48	1.40
2	A	501	PLP	C3-C4	3.89	1.48	1.40

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	PLP	C4A-C4-C5	7.48	128.64	120.94
2	B	501	PLP	C4A-C4-C5	7.33	128.49	120.94
2	B	501	PLP	C3-C4-C5	-4.05	114.37	118.74
2	A	501	PLP	C3-C4-C5	-3.80	114.64	118.74
2	A	501	PLP	C4A-C4-C3	-2.33	116.56	120.50
2	A	501	PLP	O4P-P-O1P	-2.19	100.32	106.47
2	B	501	PLP	C6-N1-C2	2.12	123.09	119.17
2	A	501	PLP	C6-C5-C4	2.11	119.82	118.16
2	B	501	PLP	C4A-C4-C3	-2.05	117.03	120.50
2	A	501	PLP	C6-N1-C2	2.03	122.93	119.17

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	504	PEG	O2-C3-C4-O4
4	A	505	PEG	O2-C3-C4-O4
4	A	504	PEG	O1-C1-C2-O2
4	B	503	PEG	O2-C3-C4-O4
4	A	504	PEG	C1-C2-O2-C3

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	455/479 (94%)	-0.10	18 (3%) 38 44	16, 23, 52, 74	0
1	B	454/479 (94%)	0.15	20 (4%) 34 40	17, 28, 59, 77	0
All	All	909/958 (94%)	0.02	38 (4%) 36 42	16, 26, 55, 77	0

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	392	GLY	5.5
1	A	393	ALA	5.4
1	B	400	ALA	5.3
1	B	390	ASP	4.1
1	B	401	LEU	4.1
1	A	401	LEU	3.8
1	A	395	THR	3.6
1	B	194	GLY	3.6
1	B	192	PRO	3.6
1	B	393	ALA	3.5
1	B	193	PRO	3.4
1	B	191	ALA	3.3
1	B	392	GLY	3.1
1	A	4	LEU	3.1
1	A	6	GLN	3.1
1	A	389	ALA	3.0
1	B	398	ASP	3.0
1	B	394	ARG	2.8
1	A	390	ASP	2.8
1	A	3	SER	2.7
1	B	451	PHE	2.7
1	B	368	GLY	2.7
1	A	396	PRO	2.6
1	A	191	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	5	GLU	2.5
1	A	397	PHE	2.5
1	B	396	PRO	2.5
1	A	398	ASP	2.4
1	A	394	ARG	2.4
1	B	46	HIS	2.4
1	A	46	HIS	2.4
1	A	400	ALA	2.4
1	B	395	THR	2.3
1	B	397	PHE	2.3
1	A	372	LEU	2.2
1	B	47	GLU	2.1
1	B	454	VAL	2.1
1	A	194	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 ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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
4	PEG	A	505	7/7	0.80	0.14	41,43,45,45	0
2	PLP	A	501	15/16	0.88	0.26	22,25,26,26	15
4	PEG	A	504	7/7	0.91	0.13	27,29,35,37	0
4	PEG	B	503	7/7	0.91	0.13	37,37,41,42	0
2	PLP	B	501	15/16	0.91	0.29	24,26,27,29	15
3	CA	B	502	1/1	0.95	0.05	52,52,52,52	0
3	CA	A	503	1/1	0.96	0.06	30,30,30,30	0
3	CA	A	502	1/1	0.99	0.03	27,27,27,27	0

6.5 Other polymers [i](#)

There are no such residues in this entry.