Full wwPDB X-ray Structure Validation Report (i)

Aug 20, 2023 – 05:37 PM EDT

PDB ID	:	2I5X
Title	:	Engineering the PTPbeta catalytic domain with improved crystallization properties
Authors	:	Evdokimov, A.G.; Pokross, M.E.; Walter, R.L.; Mekel, M.; Klopfenstein, S.
Deposited on	:	2006-08-26
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 (i) 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 (i)) were used in the production of this report:

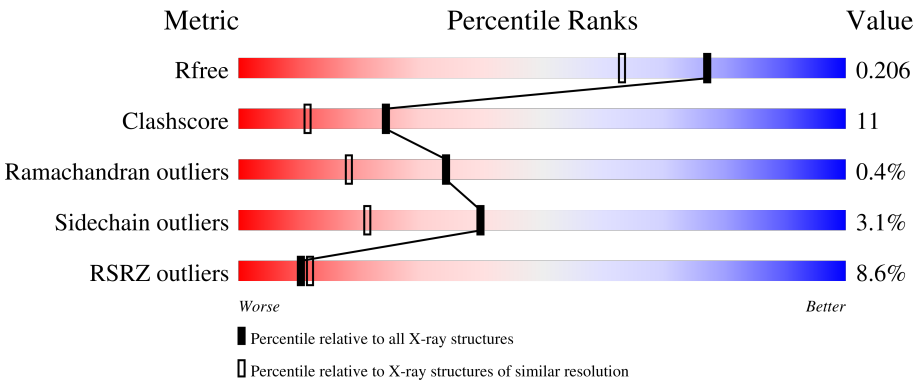
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

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}	130704	4298 (1.70-1.70)
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)
RSRZ outliers	127900	4222 (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 <=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	313	6% 73% 15% • 11%
1	B	313	9% 72% 15% • 10%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	CL	A	602	-	-	X	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 5018 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 Receptor-type tyrosine-protein phosphatase beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	280	2331	1480	415	420	16	0	9	0
1	B	281	2332	1480	416	421	15	0	8	0

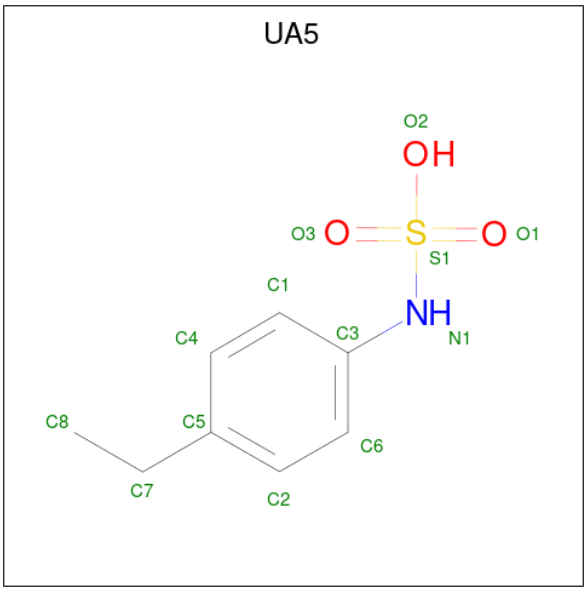
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1661	SER	-	cloning artifact	UNP P23467
B	1661	SER	-	cloning artifact	UNP P23467

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 3 is (4-ETHYLPHENYL)SULFAMIC ACID (three-letter code: UA5) (formula: $C_8H_{11}NO_3S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
3	A	1	13	8	1	3	1	0	0
			Total	C	N	O	S		
3	B	1	13	8	1	3	1	0	0

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
4	B	1	1	1	0	0

- Molecule 5 is water.

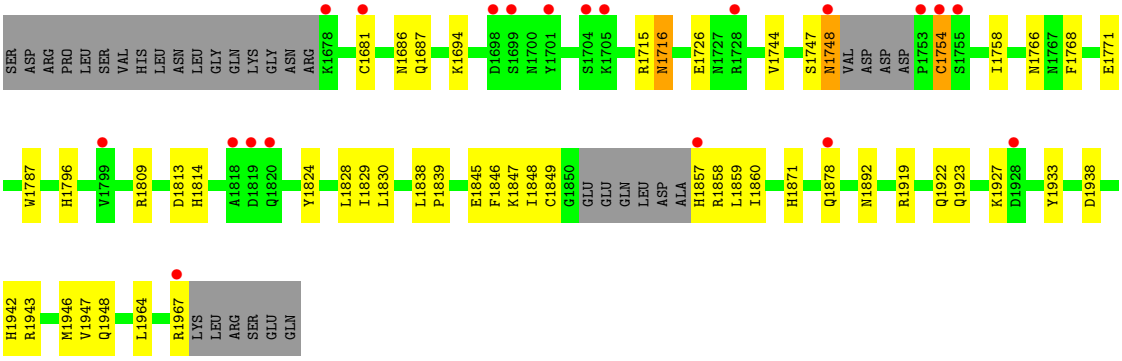
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	199	199	199	0	0
			Total	O		
5	B	127	127	127	0	0

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.

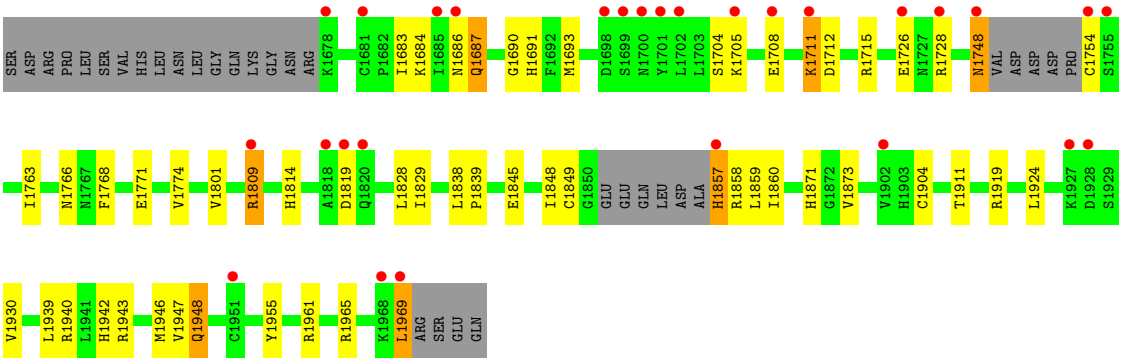
• Molecule 1: Receptor-type tyrosine-protein phosphatase beta

Chain A:



• Molecule 1: Receptor-type tyrosine-protein phosphatase beta

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	61.97Å 71.31Å 69.69Å 90.00° 93.40° 90.00°	Depositor
Resolution (Å)	39.60 – 1.70 39.62 – 1.70	Depositor EDS
% Data completeness (in resolution range)	99.6 (39.60-1.70) 99.6 (39.62-1.70)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.01 (at 1.71Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.179 , 0.207 0.178 , 0.206	Depositor DCC
R_{free} test set	3354 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å^2)	19.0	Xtriage
Anisotropy	0.034	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 51.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	5018	wwPDB-VP
Average B, all atoms (Å^2)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.82% of the height of the origin peak. No significant pseudotranslation is detected.*

[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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: UA5, CL, MG

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	0.37	0/2413	0.50	0/3271
1	B	0.33	0/2410	0.46	0/3266
All	All	0.35	0/4823	0.48	0/6537

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 (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	2331	0	2313	51	0
1	B	2332	0	2315	52	2
2	A	1	0	0	2	0
2	B	1	0	0	0	0
3	A	13	0	11	0	0
3	B	13	0	11	0	0
4	B	1	0	0	0	0
5	A	199	0	0	11	0
5	B	127	0	0	6	2
All	All	5018	0	4650	103	2

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 11.

All (103) 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:1845:GLU:CG	1:A:1859[B]:LEU:HD21	1.65	1.22
1:A:1726:GLU:OE2	1:A:1754:CYS:HB2	1.44	1.16
1:A:1845:GLU:HG2	1:A:1859[B]:LEU:CD2	1.88	1.03
1:A:1845:GLU:HG2	1:A:1859[B]:LEU:HD21	0.99	0.97
1:B:1708:GLU:O	1:B:1711:LYS:HB2	1.70	0.92
1:A:1748:ASN:C	1:A:1748:ASN:HD22	1.70	0.92
1:B:1924:LEU:CD2	1:B:1930[B]:VAL:HG21	2.01	0.91
1:A:1716:ASN:HB3	5:A:448:HOH:O	1.73	0.87
1:B:1766:ASN:ND2	5:B:217:HOH:O	2.05	0.87
1:A:1726:GLU:OE2	1:A:1754:CYS:CB	2.24	0.84
1:B:1828:LEU:HD13	1:B:1848:ILE:HD11	1.59	0.84
1:A:1919:ARG:NH1	5:A:309:HOH:O	2.11	0.83
1:B:1871:HIS:HD2	1:B:1948:GLN:HE22	1.23	0.82
1:B:1924:LEU:HD21	1:B:1930[B]:VAL:HG21	1.62	0.82
1:B:1924:LEU:HD23	1:B:1930[B]:VAL:CG2	2.12	0.80
1:A:1748:ASN:C	1:A:1748:ASN:ND2	2.37	0.78
1:A:1716:ASN:H	1:A:1716:ASN:HD22	1.32	0.77
1:A:1813:ASP:OD1	5:A:190:HOH:O	2.06	0.74
1:A:1828:LEU:HD13	1:A:1848:ILE:HD11	1.69	0.73
1:B:1924:LEU:HD23	1:B:1930[B]:VAL:HG21	1.70	0.72
1:B:1858:ARG:HD2	1:B:1860:ILE:HD11	1.72	0.70
1:A:1787:TRP:CZ2	1:A:1830[A]:LEU:HD11	2.27	0.70
1:B:1871:HIS:HD2	1:B:1948:GLN:NE2	1.89	0.69
1:B:1919:ARG:NH2	5:B:217:HOH:O	2.19	0.65
1:B:1838:LEU:HB3	1:B:1839:PRO:CD	2.28	0.63
1:B:1684:LYS:HB2	1:B:1687:GLN:HB2	1.81	0.63
1:A:1716:ASN:H	1:A:1716:ASN:ND2	1.98	0.62
1:B:1766:ASN:ND2	1:B:1919:ARG:HE	1.98	0.62
1:B:1857:HIS:N	1:B:1857:HIS:CD2	2.68	0.62
1:A:1747:SER:O	1:A:1748:ASN:CG	2.39	0.61
1:B:1871:HIS:CD2	1:B:1948:GLN:HE22	2.13	0.61
1:A:1796:HIS:CD2	1:A:1858:ARG:HD3	2.35	0.60
1:A:1747:SER:O	1:A:1748:ASN:ND2	2.33	0.60
1:B:1857:HIS:N	5:B:503:HOH:O	2.35	0.60
1:A:1829[B]:ILE:HG22	1:A:1849:CYS:HB2	1.84	0.60
1:B:1726:GLU:HG2	1:B:1754:CYS:HB2	1.83	0.59
1:B:1969:LEU:N	1:B:1969:LEU:CD1	2.65	0.58
1:A:1829[B]:ILE:CG2	1:A:1849:CYS:HB2	2.34	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1715[B]:ARG:HG2	5:A:93:HOH:O	2.04	0.57
1:A:1715[B]:ARG:NH2	5:A:87:HOH:O	2.37	0.57
1:A:1858:ARG:HD2	1:A:1860:ILE:HD11	1.86	0.57
1:B:1838:LEU:HB3	1:B:1839:PRO:HD2	1.88	0.56
1:B:1748:ASN:N	1:B:1748:ASN:OD1	2.37	0.56
1:A:1938:ASP:O	1:A:1942:HIS:HD2	1.90	0.55
1:B:1766:ASN:HD22	1:B:1919:ARG:HE	1.54	0.54
1:B:1829[A]:ILE:HG22	1:B:1849:CYS:HB2	1.89	0.54
1:B:1829[A]:ILE:CG2	1:B:1849:CYS:HB2	2.37	0.54
1:A:1923:GLN:HA	1:A:1927:LYS:HE3	1.90	0.53
1:A:1964:LEU:HD23	1:A:1967:ARG:NH1	2.25	0.51
1:A:1845:GLU:CG	1:A:1859[B]:LEU:CD2	2.60	0.51
1:A:1871:HIS:HD2	1:A:1948:GLN:OE1	1.94	0.51
1:B:1859:LEU:HD13	1:B:1860:ILE:N	2.26	0.50
1:A:1942:HIS:HE1	5:A:422:HOH:O	1.94	0.50
1:A:1847:LYS:HE3	1:A:1849:CYS:SG	2.52	0.50
1:B:1768:PHE:CE2	1:B:1771:GLU:HA	2.47	0.50
1:A:1744:VAL:O	2:A:602:CL:CL	2.66	0.49
1:B:1754:CYS:HA	5:B:179:HOH:O	2.12	0.49
1:A:1878:GLN:HB2	5:A:235:HOH:O	2.13	0.49
1:A:1686:ASN:OD1	1:A:1687:GLN:HG3	2.13	0.49
1:A:1766:ASN:ND2	1:A:1922:GLN:HB2	2.27	0.48
1:A:1768:PHE:CE2	1:A:1771:GLU:HA	2.48	0.48
1:A:1838:LEU:HB3	1:A:1839:PRO:CD	2.43	0.48
1:B:1774[A]:VAL:HG13	1:B:1911:THR:HG21	1.94	0.48
1:A:1830[A]:LEU:HD22	1:A:1846:PHE:HB3	1.94	0.48
1:B:1858:ARG:HD2	1:B:1860:ILE:CD1	2.43	0.48
1:A:1849:CYS:HG	1:A:1857:HIS:CE1	2.28	0.48
1:B:1961:ARG:HD2	1:B:1965:ARG:NH2	2.29	0.47
1:B:1712:ASP:O	1:B:1715[B]:ARG:HG2	2.14	0.47
1:A:1787:TRP:CH2	1:A:1830[A]:LEU:HD11	2.50	0.47
1:B:1763:ILE:HG21	1:B:1939:LEU:HD23	1.98	0.46
1:B:1809:ARG:HH11	1:B:1809:ARG:HG3	1.81	0.46
1:B:1857:HIS:N	1:B:1857:HIS:HD2	2.14	0.45
1:B:1940:ARG:HD2	5:B:286:HOH:O	2.15	0.45
1:A:1747:SER:O	1:A:1748:ASN:CB	2.64	0.45
1:B:1683:ILE:HG13	1:B:1691:HIS:CD2	2.52	0.44
1:A:1758:ILE:O	2:A:602:CL:CL	2.72	0.44
1:B:1924:LEU:CD2	1:B:1930[B]:VAL:CG2	2.74	0.44
1:A:1858:ARG:HD2	1:A:1860:ILE:CD1	2.48	0.44
1:A:1824:TYR:CE1	1:A:1829[A]:ILE:HG12	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1763:ILE:CG2	1:B:1939:LEU:HD23	2.47	0.43
1:B:1969:LEU:HD13	1:B:1969:LEU:H	1.83	0.43
1:A:1694:LYS:HB2	1:A:1694:LYS:HE3	1.47	0.43
1:A:1766:ASN:OD1	5:A:466:HOH:O	2.21	0.43
1:A:1892:ASN:OD1	5:A:394:HOH:O	2.21	0.43
1:A:1681[B]:CYS:HB2	1:A:1933:TYR:HB3	2.00	0.43
1:A:1814:HIS:HD2	5:A:107:HOH:O	2.01	0.43
1:A:1814:HIS:HE1	5:A:64:HOH:O	2.02	0.43
1:B:1969:LEU:N	1:B:1969:LEU:HD12	2.33	0.43
1:B:1814:HIS:HD2	5:B:199:HOH:O	2.02	0.43
1:B:1943:ARG:O	1:B:1946:MET:HG2	2.19	0.43
1:B:1859:LEU:HD13	1:B:1859:LEU:C	2.39	0.43
1:A:1824:TYR:CD1	1:A:1829[A]:ILE:HG12	2.55	0.42
1:B:1763:ILE:HG21	1:B:1939:LEU:CD2	2.50	0.42
1:B:1690:GLY:HA2	1:B:1693:MET:HE2	2.02	0.41
1:B:1774[A]:VAL:HG22	1:B:1911:THR:CG2	2.50	0.41
1:B:1801:VAL:HG23	1:B:1904:CYS:HB3	2.03	0.41
1:A:1845:GLU:CD	1:A:1859[B]:LEU:HD21	2.34	0.41
1:A:1943:ARG:O	1:A:1946:MET:HG2	2.21	0.41
1:B:1726:GLU:HB3	1:B:1754:CYS:SG	2.61	0.41
1:B:1838:LEU:HD12	1:B:1838:LEU:N	2.35	0.40
1:B:1845:GLU:OE1	1:B:1859:LEU:HD21	2.21	0.40
1:B:1873:VAL:HG11	1:B:1955:TYR:HB2	2.03	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1715[B]:ARG:NH2	5:B:340:HOH:O[2_445]	1.20	1.00
1:B:1715[B]:ARG:CZ	5:B:340:HOH:O[2_445]	1.85	0.35

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	283/313 (90%)	271 (96%)	11 (4%)	1 (0%)	34	18
1	B	283/313 (90%)	276 (98%)	6 (2%)	1 (0%)	34	18
All	All	566/626 (90%)	547 (97%)	17 (3%)	2 (0%)	34	18

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	1947	VAL
1	A	1947	VAL

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	263/284 (93%)	259 (98%)	4 (2%)	65	51
1	B	263/284 (93%)	251 (95%)	12 (5%)	27	10
All	All	526/568 (93%)	510 (97%)	16 (3%)	40	22

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1716	ASN
1	A	1748	ASN
1	A	1754	CYS
1	A	1809	ARG
1	B	1686	ASN
1	B	1687	GLN
1	B	1704	SER
1	B	1705	LYS
1	B	1711	LYS
1	B	1728	ARG
1	B	1748	ASN
1	B	1809	ARG

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Mol	Chain	Res	Type
1	B	1819	ASP
1	B	1857	HIS
1	B	1948	GLN
1	B	1969	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1716	ASN
1	A	1748	ASN
1	A	1796	HIS
1	A	1814	HIS
1	A	1871	HIS
1	A	1942	HIS
1	B	1686	ASN
1	B	1717	GLN
1	B	1734	ASN
1	B	1766	ASN
1	B	1814	HIS
1	B	1871	HIS
1	B	1942	HIS
1	B	1945	HIS
1	B	1948	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 5 ligands modelled in this entry, 3 are monoatomic - leaving 2 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	$\#\|Z\| > 2$
3	UA5	B	702	-	12,13,13	2.57	3 (25%)	12,18,18	1.22	1 (8%)
3	UA5	A	701	-	12,13,13	2.47	3 (25%)	12,18,18	1.26	1 (8%)

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	UA5	B	702	-	-	0/7/7/7	0/1/1/1
3	UA5	A	701	-	-	0/7/7/7	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	702	UA5	O1-S1	5.86	1.48	1.42
3	A	701	UA5	O3-S1	5.38	1.48	1.42
3	A	701	UA5	O1-S1	5.02	1.47	1.42
3	B	702	UA5	O3-S1	4.80	1.47	1.42
3	B	702	UA5	C3-N1	-4.43	1.35	1.43
3	A	701	UA5	C3-N1	-4.13	1.36	1.43

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	701	UA5	O3-S1-O1	-4.05	110.58	120.16
3	B	702	UA5	O3-S1-O1	-3.89	110.97	120.16

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 (i)

6.1 Protein, DNA and RNA chains (i)

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	280/313 (89%)	0.40	20 (7%)	16	18	10, 18, 36, 51	0
1	B	281/313 (89%)	0.57	28 (9%)	7	8	12, 21, 41, 57	0
All	All	561/626 (89%)	0.49	48 (8%)	10	12	10, 20, 38, 57	0

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1753	PRO	8.6
1	B	1701	TYR	6.6
1	A	1754	CYS	6.2
1	B	1754	CYS	6.0
1	A	1748	ASN	5.9
1	A	1857	HIS	5.8
1	A	1678	LYS	5.7
1	B	1748	ASN	5.0
1	B	1857	HIS	4.6
1	B	1699	SER	4.6
1	B	1705	LYS	4.4
1	A	1701	TYR	4.1
1	B	1969	LEU	3.9
1	B	1818	ALA	3.9
1	B	1728	ARG	3.7
1	A	1728	ARG	3.6
1	B	1698	ASP	3.6
1	B	1726	GLU	3.5
1	A	1819	ASP	3.5
1	A	1928	ASP	2.9
1	B	1711	LYS	2.8
1	A	1967	ARG	2.8
1	A	1818	ALA	2.6
1	A	1878	GLN	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	1681	CYS	2.5
1	B	1708	GLU	2.4
1	B	1702	LEU	2.4
1	A	1820	GLN	2.4
1	B	1968	LYS	2.3
1	B	1928	ASP	2.3
1	B	1820	GLN	2.3
1	A	1699	SER	2.3
1	A	1704	SER	2.3
1	B	1927	LYS	2.3
1	A	1698	ASP	2.3
1	B	1686	ASN	2.3
1	B	1685	ILE	2.2
1	A	1755	SER	2.2
1	B	1819	ASP	2.2
1	A	1705	LYS	2.2
1	B	1951	CYS	2.1
1	B	1755	SER	2.1
1	A	1799	VAL	2.1
1	B	1902	VAL	2.1
1	A	1681[A]	CYS	2.1
1	B	1700	ASN	2.0
1	B	1809	ARG	2.0
1	B	1678	LYS	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 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, 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
2	CL	B	603	1/1	0.95	0.07	32,32,32,32	0
4	MG	B	601	1/1	0.96	0.16	28,28,28,28	0
3	UA5	B	702	13/13	0.97	0.09	16,20,26,33	0
2	CL	A	602	1/1	0.98	0.14	26,26,26,26	0
3	UA5	A	701	13/13	0.99	0.07	13,17,23,31	0

6.5 Other polymers (i)

There are no such residues in this entry.