



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:20 AM UTC

PDB ID : 6JV9 / pdb_00006jv9
Title : Crystal Structure of Human CRMP2 1-532, unmodified
Authors : Jiang, X.; Ogawa, T.; Hirokawa, N.
Deposited on : 2019-04-16
Resolution : 2.26 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

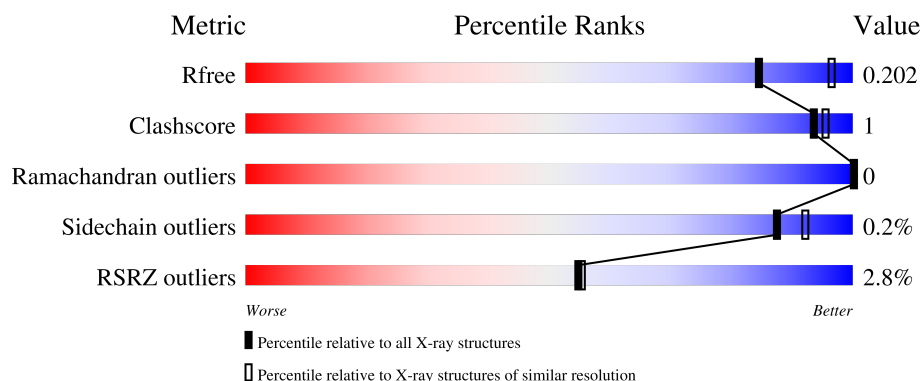
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.26 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	1898 (2.26-2.26)
Clashscore	190562	2005 (2.26-2.26)
Ramachandran outliers	187476	1965 (2.26-2.26)
Sidechain outliers	187428	1966 (2.26-2.26)
RSRZ outliers	180081	1898 (2.26-2.26)

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	540	0% 86% 10%
1	B	540	3% 87% 8%
1	C	540	3% 85% 11%
1	D	540	3% 86% 11%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 15486 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 Dihydropyrimidinase-related protein 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	486	Total	C	N	O	S	0	0	0
			3729	2349	638	724	18			
1	B	495	Total	C	N	O	S	0	0	0
			3771	2377	646	729	19			
1	C	483	Total	C	N	O	S	0	0	0
			3691	2324	634	715	18			
1	D	483	Total	C	N	O	S	0	0	0
			3692	2325	634	715	18			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	MET	-	initiating methionine	UNP Q16555
A	-6	HIS	-	expression tag	UNP Q16555
A	-5	HIS	-	expression tag	UNP Q16555
A	-4	HIS	-	expression tag	UNP Q16555
A	-3	HIS	-	expression tag	UNP Q16555
A	-2	HIS	-	expression tag	UNP Q16555
A	-1	HIS	-	expression tag	UNP Q16555
A	0	HIS	-	expression tag	UNP Q16555
B	-7	MET	-	initiating methionine	UNP Q16555
B	-6	HIS	-	expression tag	UNP Q16555
B	-5	HIS	-	expression tag	UNP Q16555
B	-4	HIS	-	expression tag	UNP Q16555
B	-3	HIS	-	expression tag	UNP Q16555
B	-2	HIS	-	expression tag	UNP Q16555
B	-1	HIS	-	expression tag	UNP Q16555
B	0	HIS	-	expression tag	UNP Q16555
C	-7	MET	-	initiating methionine	UNP Q16555
C	-6	HIS	-	expression tag	UNP Q16555
C	-5	HIS	-	expression tag	UNP Q16555
C	-4	HIS	-	expression tag	UNP Q16555
C	-3	HIS	-	expression tag	UNP Q16555

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	-2	HIS	-	expression tag	UNP Q16555
C	-1	HIS	-	expression tag	UNP Q16555
C	0	HIS	-	expression tag	UNP Q16555
D	-7	MET	-	initiating methionine	UNP Q16555
D	-6	HIS	-	expression tag	UNP Q16555
D	-5	HIS	-	expression tag	UNP Q16555
D	-4	HIS	-	expression tag	UNP Q16555
D	-3	HIS	-	expression tag	UNP Q16555
D	-2	HIS	-	expression tag	UNP Q16555
D	-1	HIS	-	expression tag	UNP Q16555
D	0	HIS	-	expression tag	UNP Q16555

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

- Molecule 3 is 2,3-DIHYDROXY-1,4-DITHIOBUTANE (CCD ID: DTT) (formula: C₄H₁₀O₂S₂).



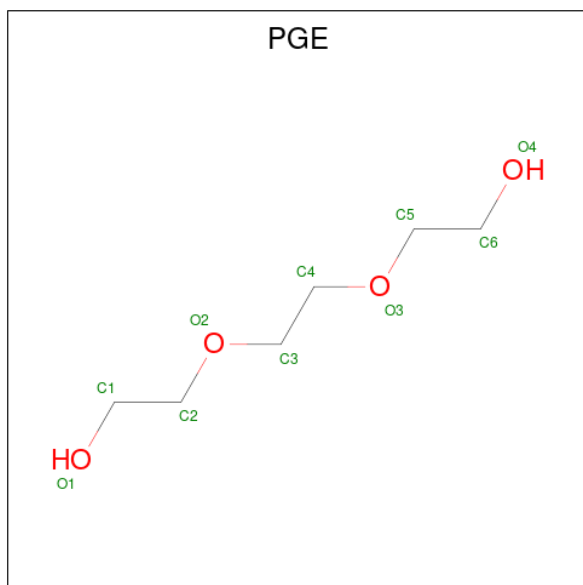
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	O	S	0	0
			8	4	2	2		

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



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

- Molecule 5 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: $C_6H_{14}O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	D	1	Total	C	O	0	0
			10	6	4		

- Molecule 6 is water.

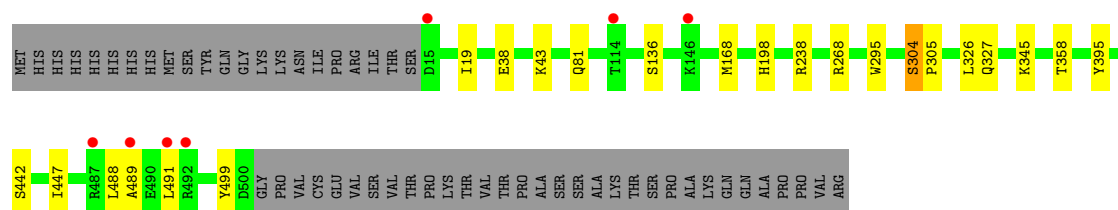
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	162	Total	O	0	0
			162	162		
6	B	170	Total	O	0	0
			170	170		
6	C	133	Total	O	0	0
			133	133		
6	D	106	Total	O	0	0
			106	106		

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.

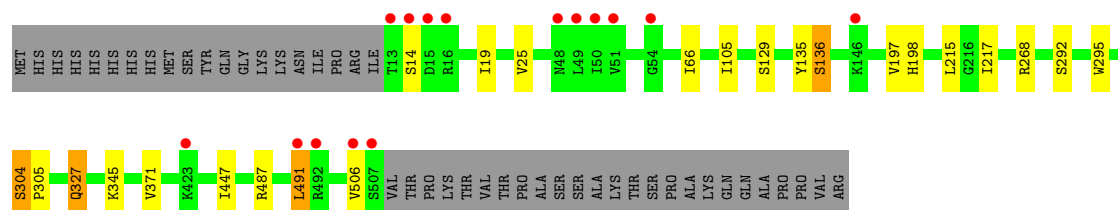
• Molecule 1: Dihydropyrimidinase-related protein 2

Chain A: 



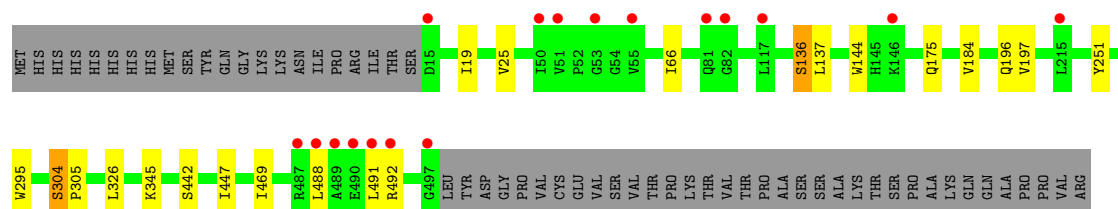
• Molecule 1: Dihydropyrimidinase-related protein 2

Chain B: 



• Molecule 1: Dihydropyrimidinase-related protein 2

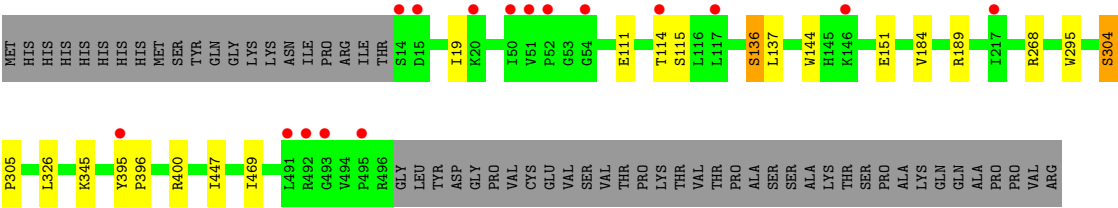
Chain C: 



• Molecule 1: Dihydropyrimidinase-related protein 2

Chain D: 





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	80.09Å 158.43Å 88.00Å 90.00° 94.19° 90.00°	Depositor
Resolution (Å)	50.00 – 2.26 50.00 – 2.26	Depositor EDS
% Data completeness (in resolution range)	99.7 (50.00-2.26) 99.8 (50.00-2.26)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.97 (at 2.27Å)	Xtriage
Refinement program	REFMAC 5.8.0135, REFMAC	Depositor
R, R_{free}	0.171 , 0.193 0.180 , 0.202	Depositor DCC
R_{free} test set	5112 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	26.7	Xtriage
Anisotropy	0.304	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 28.4	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	0.95	EDS
Total number of atoms	15486	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.50% 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](#)

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

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	1.05	4/3806 (0.1%)	1.00	7/5167 (0.1%)
1	B	1.08	5/3849 (0.1%)	1.02	6/5228 (0.1%)
1	C	1.05	1/3767 (0.0%)	1.00	7/5114 (0.1%)
1	D	1.04	2/3768 (0.1%)	0.99	3/5116 (0.1%)
All	All	1.05	12/15190 (0.1%)	1.00	23/20625 (0.1%)

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	358	THR	C-O	-6.57	1.16	1.24
1	B	197	VAL	C-O	-6.24	1.17	1.24
1	B	268	ARG	C-O	-6.00	1.17	1.24
1	D	268	ARG	C-O	-5.85	1.17	1.24
1	B	304	SER	C-O	-5.79	1.16	1.24
1	A	304	SER	C-O	-5.77	1.16	1.24
1	B	487	ARG	C-O	-5.76	1.16	1.24
1	A	395	TYR	C-O	-5.56	1.15	1.24
1	B	129	SER	C-O	-5.44	1.16	1.24
1	D	189	ARG	C-O	-5.23	1.18	1.24
1	C	197	VAL	C-O	-5.14	1.18	1.24
1	A	268	ARG	C-O	-5.04	1.18	1.24

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	304	SER	C-N-CD	7.18	136.40	120.60
1	B	14	SER	N-CA-C	6.85	119.64	108.55
1	B	304	SER	C-N-CD	6.75	135.45	120.60
1	A	304	SER	C-N-CD	6.70	135.33	120.60
1	D	304	SER	C-N-CD	6.60	135.11	120.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	491	LEU	N-CA-C	-6.41	99.58	109.76
1	C	492	ARG	N-CA-C	6.35	121.37	112.93
1	C	137	LEU	N-CA-C	6.21	119.26	108.76
1	C	175	GLN	N-CA-C	6.21	119.36	110.24
1	C	326	LEU	N-CA-C	-5.94	99.22	108.90
1	B	198	HIS	N-CA-C	-5.85	98.19	108.20
1	D	137	LEU	N-CA-C	5.75	118.48	108.76
1	A	488	LEU	N-CA-C	5.64	117.51	111.36
1	A	326	LEU	N-CA-C	-5.63	99.24	108.76
1	B	135	TYR	N-CA-C	5.61	117.59	109.07
1	B	327	GLN	N-CA-C	5.58	120.74	113.88
1	A	442	SER	N-CA-C	5.53	113.20	108.22
1	B	491	LEU	N-CA-C	-5.48	102.29	110.23
1	A	198	HIS	N-CA-C	-5.21	98.06	107.75
1	A	327	GLN	N-CA-C	5.20	120.28	113.88
1	C	442	SER	N-CA-C	5.18	112.88	108.22
1	A	499	TYR	N-CA-C	5.17	118.00	109.72
1	D	326	LEU	N-CA-C	-5.16	100.48	108.90

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	3729	0	3658	10	0
1	B	3771	0	3692	15	0
1	C	3691	0	3617	8	0
1	D	3692	0	3616	14	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
3	B	8	0	10	1	0
4	C	4	0	6	0	0
5	D	10	0	14	0	0
6	A	162	0	0	0	0
6	B	170	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	C	133	0	0	0	0
6	D	106	0	0	0	0
All	All	15486	0	14613	42	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 (42) 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:395:TYR:OH	1:D:400:ARG:HD2	1.88	0.74
1:B:491:LEU:HD12	1:B:491:LEU:H	1.57	0.67
1:D:304:SER:HA	1:D:305:PRO:C	2.18	0.67
1:B:105:ILE:HG23	1:B:136:SER:HB3	1.77	0.66
1:A:491:LEU:HB3	1:B:217:ILE:HD11	1.81	0.62
1:D:111:GLU:O	1:D:114:THR:OG1	2.20	0.59
1:B:491:LEU:HD12	1:B:491:LEU:N	2.24	0.53
1:D:395:TYR:CD1	1:D:396:PRO:HA	2.44	0.52
1:A:491:LEU:HB3	1:B:217:ILE:CD1	2.41	0.51
1:A:489:ALA:O	1:A:491:LEU:HD22	2.11	0.50
1:D:395:TYR:CG	1:D:396:PRO:HA	2.47	0.50
1:A:38:GLU:HG2	1:A:43:LYS:HG3	1.95	0.49
1:B:292:SER:OG	3:B:601:DTT:H12	2.12	0.49
1:A:304:SER:HA	1:A:305:PRO:C	2.38	0.48
1:D:115:SER:OG	1:D:151:GLU:OE1	2.31	0.47
1:A:295:TRP:CZ2	1:A:345:LYS:HA	2.50	0.47
1:D:395:TYR:CZ	1:D:396:PRO:HB3	2.50	0.46
1:B:327:GLN:N	1:B:327:GLN:CD	2.73	0.46
1:C:304:SER:HA	1:C:305:PRO:C	2.40	0.46
1:D:395:TYR:CZ	1:D:400:ARG:HD2	2.49	0.46
1:C:136:SER:OG	1:C:469:ILE:O	2.31	0.46
1:C:295:TRP:CZ2	1:C:345:LYS:HA	2.50	0.46
1:D:295:TRP:CZ2	1:D:345:LYS:HA	2.52	0.45
1:B:295:TRP:CZ2	1:B:345:LYS:HA	2.51	0.45
1:D:136:SER:OG	1:D:469:ILE:O	2.35	0.45
1:A:491:LEU:HB2	1:B:215:LEU:HD13	1.98	0.44
1:D:395:TYR:OH	1:D:400:ARG:CD	2.63	0.44
1:A:168:MET:HE2	1:A:238:ARG:NH1	2.34	0.43
1:B:371:VAL:O	1:C:488:LEU:HD11	2.19	0.42
1:B:304:SER:HA	1:B:305:PRO:C	2.44	0.42
1:D:395:TYR:CE2	1:D:396:PRO:HB3	2.54	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:25:VAL:HB	1:C:66:ILE:HG22	2.01	0.41
1:C:144:TRP:CE3	1:C:184:VAL:HG22	2.55	0.41
1:C:196:GLN:HG2	1:C:251:TYR:CD1	2.54	0.41
1:D:19:ILE:HD11	1:D:447:ILE:CD1	2.50	0.41
1:A:81:GLN:O	1:B:506:VAL:HG13	2.20	0.41
1:B:25:VAL:HB	1:B:66:ILE:HG22	2.03	0.41
1:B:491:LEU:H	1:B:491:LEU:CD1	2.29	0.41
1:C:19:ILE:HD11	1:C:447:ILE:CD1	2.50	0.41
1:D:144:TRP:CE3	1:D:184:VAL:HG22	2.56	0.41
1:A:19:ILE:HD11	1:A:447:ILE:CD1	2.51	0.40
1:B:19:ILE:HD11	1:B:447:ILE:CD1	2.51	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	484/540 (90%)	471 (97%)	13 (3%)	0	100	100
1	B	493/540 (91%)	479 (97%)	14 (3%)	0	100	100
1	C	481/540 (89%)	468 (97%)	13 (3%)	0	100	100
1	D	481/540 (89%)	465 (97%)	16 (3%)	0	100	100
All	All	1939/2160 (90%)	1883 (97%)	56 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	403/455 (89%)	402 (100%)	1 (0%)	87	92
1	B	405/455 (89%)	404 (100%)	1 (0%)	87	92
1	C	397/455 (87%)	396 (100%)	1 (0%)	86	90
1	D	397/455 (87%)	396 (100%)	1 (0%)	86	90
All	All	1602/1820 (88%)	1598 (100%)	4 (0%)	87	92

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	136	SER
1	B	136	SER
1	C	136	SER
1	D	136	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	122	GLN
1	A	237	ASN
1	A	244	ASN
1	B	91	GLN
1	B	122	GLN
1	B	198	HIS
1	B	244	ASN
1	B	245	GLN
1	C	91	GLN
1	C	122	GLN
1	C	198	HIS
1	C	210	GLN
1	C	244	ASN
1	C	449	GLN
1	D	29	GLN
1	D	91	GLN
1	D	122	GLN
1	D	198	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](#)

5 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	EDO	C	601	-	3,3,3	0.52	0	2,2,2	0.20	0
3	DTT	B	601	-	7,7,7	0.31	0	4,8,8	0.49	0
5	PGE	D	601	-	9,9,9	0.65	0	8,8,8	0.44	0
2	SO4	A	601	-	4,4,4	0.42	0	6,6,6	0.07	0
2	SO4	B	602	-	4,4,4	0.45	0	6,6,6	0.21	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
5	PGE	D	601	-	-	4/7/7/7	-
4	EDO	C	601	-	-	1/1/1/1	-
3	DTT	B	601	-	-	6/8/8/8	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	601	DTT	C1-C2-C3-O3
3	B	601	DTT	C1-C2-C3-C4
3	B	601	DTT	O2-C2-C3-O3
3	B	601	DTT	O2-C2-C3-C4
3	B	601	DTT	C2-C3-C4-S4
3	B	601	DTT	O3-C3-C4-S4
5	D	601	PGE	O3-C5-C6-O4
5	D	601	PGE	C1-C2-O2-C3
5	D	601	PGE	O1-C1-C2-O2
5	D	601	PGE	C6-C5-O3-C4
4	C	601	EDO	O1-C1-C2-O2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	601	DTT	1	0

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	486/540 (90%)	-0.22	7 (1%) 73 74	16, 25, 46, 64	0
1	B	495/540 (91%)	-0.11	15 (3%) 52 53	17, 26, 49, 67	0
1	C	483/540 (89%)	-0.01	17 (3%) 47 47	18, 30, 56, 92	0
1	D	483/540 (89%)	0.10	16 (3%) 49 49	18, 32, 55, 87	0
All	All	1947/2160 (90%)	-0.06	55 (2%) 55 55	16, 28, 52, 92	0

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	15	ASP	4.9
1	C	491	LEU	4.7
1	B	14	SER	4.7
1	C	489	ALA	4.6
1	C	81	GLN	4.3
1	D	114	THR	4.3
1	A	114	THR	4.0
1	A	491	LEU	4.0
1	D	50	ILE	3.9
1	B	13	THR	3.7
1	C	490	GLU	3.6
1	B	48	ASN	3.6
1	C	15	ASP	3.6
1	B	51	VAL	3.5
1	B	506	VAL	3.5
1	A	492	ARG	3.4
1	B	54	GLY	3.4
1	D	495	PRO	3.2
1	B	507	SER	3.2
1	D	52	PRO	3.1
1	B	50	ILE	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	15	ASP	3.0
1	D	51	VAL	3.0
1	C	53	GLY	2.9
1	D	395	TYR	2.9
1	B	491	LEU	2.9
1	A	489	ALA	2.8
1	D	146	LYS	2.8
1	D	20	LYS	2.7
1	A	146	LYS	2.7
1	B	146	LYS	2.7
1	C	492	ARG	2.7
1	D	14	SER	2.6
1	C	488	LEU	2.6
1	C	497	GLY	2.6
1	C	50	ILE	2.6
1	B	49	LEU	2.5
1	D	117	LEU	2.5
1	B	492	ARG	2.5
1	C	117	LEU	2.5
1	A	487	ARG	2.4
1	C	51	VAL	2.3
1	C	487	ARG	2.3
1	C	146	LYS	2.3
1	D	491	LEU	2.2
1	D	217	ILE	2.2
1	A	15	ASP	2.2
1	C	55	VAL	2.2
1	B	16	ARG	2.1
1	D	54	GLY	2.1
1	D	493	GLY	2.1
1	C	215	LEU	2.1
1	C	82	GLY	2.1
1	D	492	ARG	2.1
1	B	423	LYS	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](#)

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($\text{\AA}^2$)	Q<0.9
3	DTT	B	601	8/8	0.69	0.22	48,56,68,77	0
5	PGE	D	601	10/10	0.77	0.17	48,55,59,59	0
2	SO4	B	602	5/5	0.81	0.14	66,68,74,80	0
4	EDO	C	601	4/4	0.85	0.23	37,40,44,45	0
2	SO4	A	601	5/5	0.90	0.21	30,30,30,30	0

6.5 Other polymers [i](#)

There are no such residues in this entry.