



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 02:22 pm GMT

PDB ID : 4QJ0
Title : Crystal structure of catalytic domain of human carbonic anhydrase isozyme XII with inhibitor
Authors : Manakova, E.; Smirnov, A.; Grazulis, S.
Deposited on : 2014-06-03
Resolution : 1.55 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

<http://wwpdb.org/validation/2016/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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

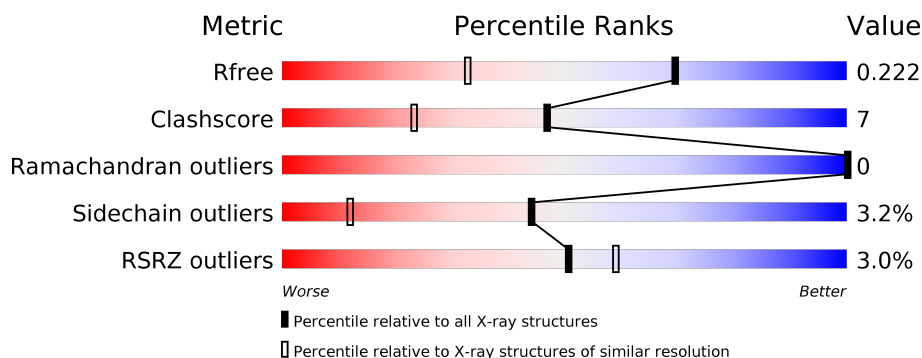
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.55 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}	100719	1088 (1.56-1.56)
Clashscore	112137	1132 (1.56-1.56)
Ramachandran outliers	110173	1110 (1.56-1.56)
Sidechain outliers	110143	1108 (1.56-1.56)
RSRZ outliers	101464	1089 (1.56-1.56)

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. 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	263	<div> <div style="width: 100%; height: 10px; position: relative;"> <div style="position: absolute; top: -10px; left: 0; width: 100%; height: 10px; background-color: red;"></div> <div style="position: absolute; bottom: 0; left: 0; width: 100%; height: 10px; background-color: green;"></div> <div style="position: absolute; top: 0; left: 0; width: 100%; height: 10px; background-color: yellow;"></div> <div style="position: absolute; top: 0; left: 100%; width: 100%; height: 10px; background-color: grey;"></div> </div> <div> % 87% 11% .. </div> </div>
1	B	263	<div> <div style="width: 100%; height: 10px; position: relative;"> <div style="position: absolute; top: -10px; left: 0; width: 100%; height: 10px; background-color: red;"></div> <div style="position: absolute; bottom: 0; left: 0; width: 100%; height: 10px; background-color: green;"></div> <div style="position: absolute; top: 0; left: 0; width: 100%; height: 10px; background-color: yellow;"></div> <div style="position: absolute; top: 0; left: 100%; width: 100%; height: 10px; background-color: grey;"></div> </div> <div> 2% 89% 10% . </div> </div>
1	C	263	<div> <div style="width: 100%; height: 10px; position: relative;"> <div style="position: absolute; top: -10px; left: 0; width: 100%; height: 10px; background-color: red;"></div> <div style="position: absolute; bottom: 0; left: 0; width: 100%; height: 10px; background-color: green;"></div> <div style="position: absolute; top: 0; left: 0; width: 100%; height: 10px; background-color: yellow;"></div> <div style="position: absolute; top: 0; left: 100%; width: 100%; height: 10px; background-color: grey;"></div> </div> <div> 8% 78% 18% .. </div> </div>
1	D	263	<div> <div style="width: 100%; height: 10px; position: relative;"> <div style="position: absolute; top: -10px; left: 0; width: 100%; height: 10px; background-color: red;"></div> <div style="position: absolute; bottom: 0; left: 0; width: 100%; height: 10px; background-color: green;"></div> <div style="position: absolute; top: 0; left: 0; width: 100%; height: 10px; background-color: yellow;"></div> <div style="position: absolute; top: 0; left: 100%; width: 100%; height: 10px; background-color: grey;"></div> </div> <div> 90% 8% .. </div> </div>

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	EDO	D	302	-	-	-	X
3	EDO	D	304	-	-	-	X
4	WWX	A	303	-	-	-	X
4	WWX	B	303	-	-	-	X
4	WWX	D	305[A]	-	-	-	X
4	WWX	D	305[B]	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 9838 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 Carbonic anhydrase 12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	260	Total	C	N	O	S	0	6	0
			2133	1354	364	407	8			
1	B	261	Total	C	N	O	S	0	6	0
			2150	1365	368	410	7			
1	C	260	Total	C	N	O	S	0	8	0
			2150	1364	365	413	8			
1	D	260	Total	C	N	O	S	0	9	0
			2160	1368	368	417	7			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	EXPRESSION TAG	UNP O43570
B	1	MET	-	EXPRESSION TAG	UNP O43570
C	1	MET	-	EXPRESSION TAG	UNP O43570
D	1	MET	-	EXPRESSION TAG	UNP O43570

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

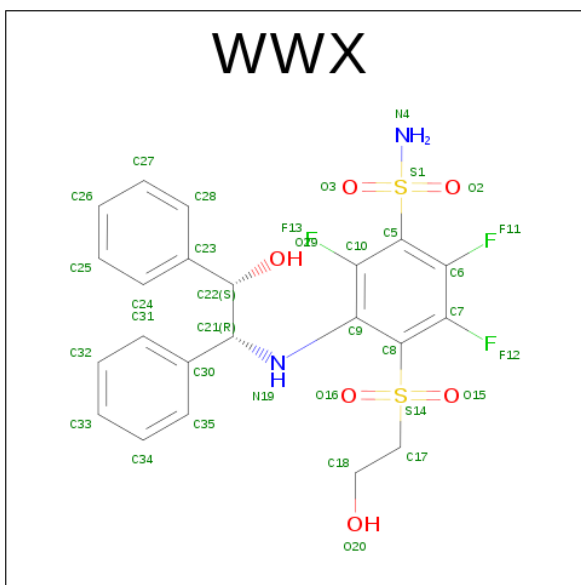
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Zn	0	0
			1	1		
2	A	1	Total	Zn	0	0
			1	1		
2	D	1	Total	Zn	0	0
			1	1		
2	C	1	Total	Zn	0	0
			1	1		

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



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

- Molecule 4 is 2,3,6-TRIFLUORO-5-[(1R,2S)-2-HYDROXY-1,2-DIPHENYLETHYL]AMINO-4-[(2-HYDROXYETHYL)SULFONYL]BENZENESULFONAMIDE (three-letter code: WWX) (formula: C₂₂H₂₁F₃N₂O₆S₂).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	A	1	Total	C	F	N	O	S	0	0
			35	22	3	2	6	2		
4	B	1	Total	C	F	N	O	S	0	0
			35	22	3	2	6	2		
4	C	1	Total	C	F	N	O	S	0	0
			35	22	3	2	6	2		
4	D	1	Total	C	F	N	O	S	0	1
			70	44	6	4	12	4		

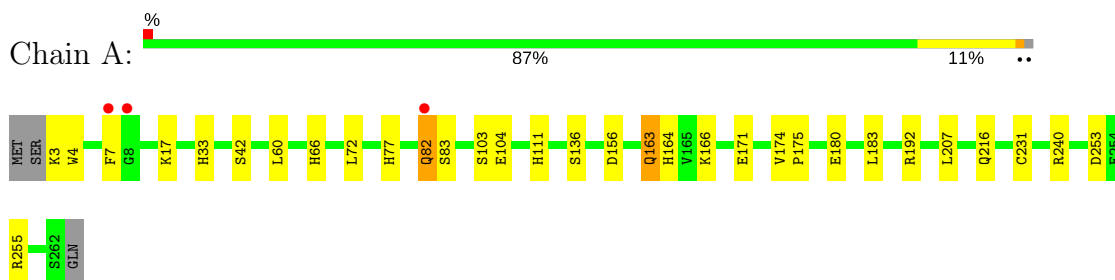
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	243	Total	O	0	0
			243	243		
5	B	290	Total	O	0	0
			290	290		
5	C	212	Total	O	0	0
			212	212		
5	D	297	Total	O	0	0
			297	297		

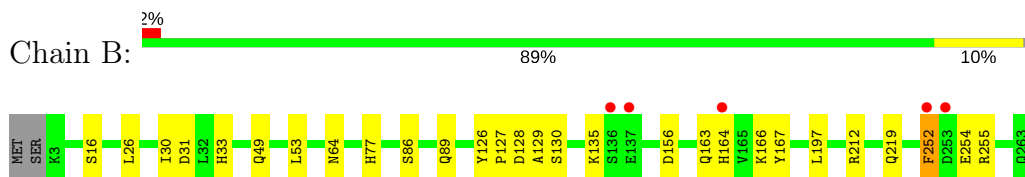
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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.

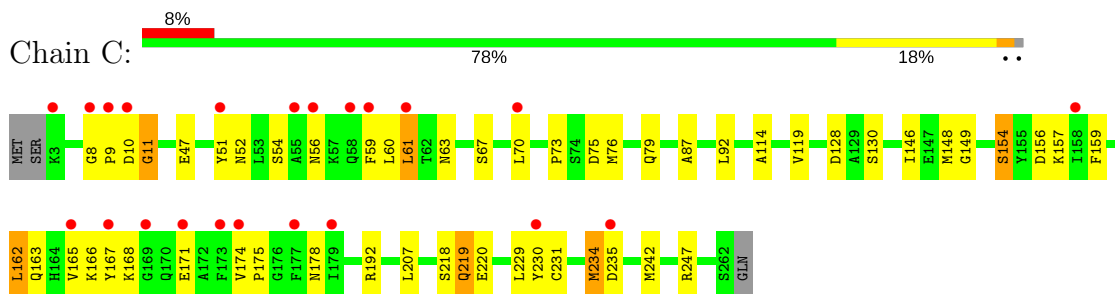
- Molecule 1: Carbonic anhydrase 12



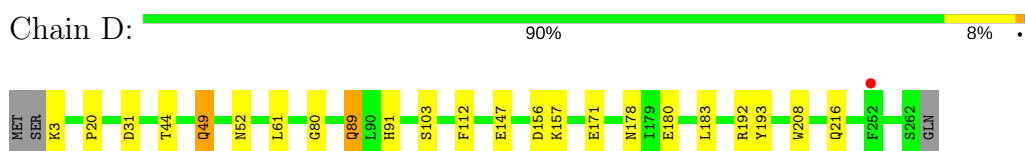
- Molecule 1: Carbonic anhydrase 12



- Molecule 1: Carbonic anhydrase 12



- Molecule 1: Carbonic anhydrase 12



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	77.51Å 74.24Å 91.42Å 90.00° 108.87° 90.00°	Depositor
Resolution (Å)	67.80 – 1.55 56.34 – 1.55	Depositor EDS
% Data completeness (in resolution range)	99.3 (67.80-1.55) 99.3 (56.34-1.55)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.15 (at 1.55Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.180 , 0.225 0.179 , 0.222	Depositor DCC
R_{free} test set	13984 reflections (11.00%)	DCC
Wilson B-factor (Å ²)	13.8	Xtriage
Anisotropy	0.466	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 38.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	9838	wwPDB-VP
Average B, all atoms (Å ²)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 50.83 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 6.1208e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: ZN, EDO, WWX

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	1.16	1/2196 (0.0%)	1.09	2/2988 (0.1%)
1	B	1.18	0/2214	1.13	3/3012 (0.1%)
1	C	1.16	3/2214 (0.1%)	1.10	1/3014 (0.0%)
1	D	1.14	2/2223 (0.1%)	1.09	4/3025 (0.1%)
All	All	1.16	6/8847 (0.1%)	1.10	10/12039 (0.1%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	208	TRP	CD2-CE2	5.98	1.48	1.41
1	C	11	GLY	N-CA	5.90	1.54	1.46
1	A	104	GLU	CD-OE1	-5.61	1.19	1.25
1	C	67	SER	CA-CB	5.16	1.60	1.52
1	C	10	ASP	C-O	5.13	1.33	1.23
1	D	103	SER	CB-OG	5.07	1.48	1.42

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	255	ARG	NE-CZ-NH2	-5.91	117.35	120.30
1	B	53	LEU	CB-CG-CD1	-5.86	101.04	111.00
1	D	31	ASP	CB-CG-OD2	5.67	123.40	118.30
1	D	112	PHE	CB-CG-CD1	-5.59	116.88	120.80
1	B	197	LEU	CB-CG-CD1	-5.53	101.60	111.00
1	A	72	LEU	CB-CG-CD1	-5.44	101.75	111.00
1	D	193	TYR	CB-CG-CD1	-5.39	117.76	121.00
1	D	157	LYS	CD-CE-NZ	5.28	123.84	111.70
1	C	247	ARG	NE-CZ-NH2	-5.16	117.72	120.30
1	B	212	ARG	NE-CZ-NH2	-5.11	117.75	120.30

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	2133	0	2023	29	0
1	B	2150	0	2035	28	0
1	C	2150	0	2026	51	0
1	D	2160	0	2034	14	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	4	0	6	0	0
3	B	4	0	6	0	0
3	C	4	0	6	0	0
3	D	12	0	18	3	0
4	A	35	0	21	0	0
4	B	35	0	21	5	0
4	C	35	0	21	1	0
4	D	70	0	42	0	0
5	A	243	0	0	8	0
5	B	290	0	0	0	0
5	C	212	0	0	1	0
5	D	297	0	0	1	0
All	All	9838	0	8259	121	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 7.

All (121) 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:61:LEU:HD21	1:C:174:VAL:CG2	1.53	1.36
1:C:61:LEU:CD2	1:C:174:VAL:HG23	1.77	1.15
1:C:61:LEU:CD2	1:C:174:VAL:CG2	2.25	1.13

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:61:LEU:HD21	1:C:174:VAL:HG21	1.06	1.03
1:A:82:GLN:HG2	1:A:83:SER:H	1.20	1.01
1:D:178:ASN:OD1	1:D:180[B]:GLU:HG2	1.63	0.98
1:C:175:PRO:HB2	5:C:509:HOH:O	1.66	0.95
1:B:31:ASP:O	1:B:252[B]:PHE:HZ	1.50	0.94
1:C:61:LEU:HD22	1:C:174:VAL:HG23	1.48	0.93
1:C:61:LEU:CD2	1:C:174:VAL:HG21	1.97	0.91
1:A:82:GLN:HG3	5:A:621:HOH:O	1.70	0.89
1:B:129:ALA:HB1	4:B:303:WWX:H12	1.54	0.89
1:A:7:PHE:CD2	5:A:638:HOH:O	2.27	0.87
1:A:7:PHE:HD2	5:A:638:HOH:O	1.60	0.83
1:B:77:HIS:CE1	1:B:86:SER:OG	2.33	0.82
1:A:216:GLN:HG3	5:A:623:HOH:O	1.78	0.82
1:A:82:GLN:HG2	1:A:83:SER:N	1.93	0.81
1:C:61:LEU:HD12	1:C:61:LEU:N	1.96	0.81
1:C:159:PHE:O	1:C:162:LEU:HG	1.83	0.78
1:C:231[A]:CYS:SG	1:C:242:MET:HA	2.23	0.78
1:C:168:LYS:HB2	1:C:231[A]:CYS:O	1.83	0.78
1:B:31:ASP:O	1:B:252[B]:PHE:CZ	2.36	0.76
1:B:252[A]:PHE:CD2	1:B:255[A]:ARG:O	2.40	0.74
1:B:77:HIS:CE1	1:B:86:SER:HG	2.06	0.74
1:B:252[A]:PHE:CE2	1:B:255[A]:ARG:O	2.41	0.74
1:C:149:GLY:O	1:C:218:SER:HA	1.88	0.73
1:B:30:ILE:HD12	1:B:252[B]:PHE:HE1	1.55	0.70
1:C:63[B]:ASN:OD1	1:C:165:VAL:HB	1.93	0.68
1:C:59:PHE:O	1:C:61:LEU:CD1	2.41	0.68
1:C:163:GLN:OE1	1:C:166:LYS:HD2	1.94	0.68
1:C:61:LEU:CD1	1:C:61:LEU:N	2.58	0.67
1:C:219:GLN:HG3	1:C:220:GLU:OE1	1.95	0.67
1:B:30:ILE:HD12	1:B:252[B]:PHE:CE1	2.29	0.66
1:B:252[A]:PHE:CE1	1:B:255[A]:ARG:HB2	2.30	0.66
1:B:129:ALA:HB1	4:B:303:WWX:C33	2.25	0.64
1:A:7:PHE:CZ	1:A:240:ARG:NH1	2.68	0.61
1:C:148:MET:SD	1:C:219:GLN:HB3	2.39	0.61
1:C:63[B]:ASN:HD21	1:C:229:LEU:HD22	1.64	0.61
1:C:63[B]:ASN:CG	1:C:165:VAL:O	2.39	0.61
1:D:49:GLN:HA	1:D:49:GLN:HE21	1.65	0.61
1:D:80:GLY:O	3:D:302:EDO:H12	2.01	0.60
1:A:77:HIS:ND1	5:A:606:HOH:O	2.32	0.60
1:C:63[B]:ASN:ND2	1:C:165:VAL:O	2.35	0.60
1:C:60:LEU:C	1:C:61:LEU:HD12	2.22	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:180[B]:GLU:HG3	5:D:599:HOH:O	2.01	0.59
1:A:82:GLN:HE21	1:A:82:GLN:H	1.51	0.59
1:C:76:MET:HB3	1:C:87:ALA:HB3	1.83	0.59
1:D:89[B]:GLN:HE21	1:D:91:HIS:HD1	1.49	0.59
1:C:61:LEU:HG	1:C:70:LEU:HD13	1.83	0.59
1:B:252[A]:PHE:CZ	1:B:255[A]:ARG:HB2	2.38	0.58
1:A:7:PHE:CZ	1:A:240:ARG:HD2	2.39	0.57
1:B:252[A]:PHE:CE2	1:B:255[A]:ARG:C	2.78	0.57
1:C:47:GLU:HB2	1:C:79:GLN:HB3	1.87	0.57
1:C:159:PHE:O	1:C:162:LEU:CD1	2.52	0.57
1:C:159:PHE:O	1:C:162:LEU:CG	2.52	0.57
1:C:167:TYR:CG	1:C:234:MET:HA	2.40	0.56
1:A:4:TRP:O	1:A:66:HIS:HE1	1.88	0.56
1:C:51:TYR:CD2	1:C:76:MET:HG2	2.41	0.56
1:D:89[B]:GLN:NE2	1:D:91:HIS:HD1	2.03	0.55
1:D:44:THR:H	3:D:302:EDO:H21	1.71	0.55
1:A:231[B]:CYS:SG	1:A:240:ARG:HB2	2.47	0.55
1:C:61:LEU:CD1	1:C:70:LEU:CD1	2.85	0.54
1:B:163:GLN:CG	1:B:164:HIS:CE1	2.91	0.54
1:B:163:GLN:HG3	1:B:164:HIS:CE1	2.43	0.54
1:C:61:LEU:HD11	1:C:174:VAL:HB	1.89	0.53
1:D:147[B]:GLU:CG	1:D:216:GLN:HG2	2.39	0.53
1:C:54:SER:HB3	1:C:56:ASN:OD1	2.09	0.53
1:A:164:HIS:HD2	5:A:581:HOH:O	1.90	0.52
1:D:180[A]:GLU:HG3	1:D:183:LEU:HD12	1.90	0.52
1:A:7:PHE:CE2	1:A:240:ARG:NH1	2.77	0.52
1:C:59:PHE:O	1:C:61:LEU:HD12	2.07	0.52
1:B:26:LEU:HA	1:B:255[A]:ARG:CZ	2.39	0.52
1:A:103:SER:O	1:A:111:HIS:HD2	1.92	0.52
1:B:166[B]:LYS:HD3	1:B:167:TYR:CZ	2.45	0.51
1:C:230[B]:TYR:CD2	1:C:230[B]:TYR:N	2.78	0.51
1:A:82:GLN:CG	1:A:83:SER:N	2.66	0.51
1:C:9:PRO:C	1:C:11:GLY:H	2.14	0.51
1:A:33:HIS:HE1	5:A:490:HOH:O	1.94	0.51
1:A:60:LEU:HD11	1:A:171:GLU:HB3	1.94	0.50
1:C:192:ARG:HD2	1:C:207:LEU:HD11	1.94	0.50
1:C:154:SER:O	1:C:157:LYS:HG3	2.11	0.50
1:B:33:HIS:HE1	1:B:252[B]:PHE:CE2	2.31	0.49
1:D:44:THR:O	3:D:302:EDO:H11	2.12	0.49
1:C:52:ASN:HA	1:C:178:ASN:HA	1.95	0.49
1:A:180:GLU:HG3	1:A:183:LEU:HD12	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:7:PHE:HZ	1:A:240:ARG:NH1	2.08	0.48
1:C:174:VAL:HG12	1:C:175:PRO:O	2.14	0.48
1:B:252[B]:PHE:O	1:B:254:GLU:N	2.43	0.48
1:C:229:LEU:C	1:C:230[B]:TYR:CD2	2.87	0.48
1:B:163:GLN:HG2	1:B:164:HIS:CE1	2.49	0.48
1:D:89[A]:GLN:OE1	1:D:91:HIS:ND1	2.39	0.47
1:D:147[B]:GLU:HG2	1:D:216:GLN:HG2	1.95	0.47
1:A:166:LYS:HE3	1:A:166:LYS:HB3	1.47	0.46
1:C:231[A]:CYS:SG	1:C:242:MET:CA	3.01	0.45
1:C:167:TYR:CD2	1:C:234:MET:HG3	2.52	0.45
1:C:60:LEU:HD11	1:C:171:GLU:HB3	1.98	0.45
1:A:17[A]:LYS:HE3	1:B:16:SER:OG	2.16	0.45
1:C:61:LEU:HD11	1:C:70:LEU:CD1	2.47	0.45
1:B:64:ASN:ND2	4:B:303:WWX:H4	2.32	0.44
1:B:126:TYR:CE1	1:B:135:LYS:HD2	2.53	0.43
1:B:252[A]:PHE:O	1:B:254:GLU:N	2.51	0.43
1:A:82:GLN:NE2	1:A:82:GLN:H	2.17	0.43
1:A:163:GLN:O	1:A:166:LYS:HG3	2.17	0.43
1:B:129:ALA:CB	4:B:303:WWX:H12	2.38	0.43
1:B:64:ASN:HD21	4:B:303:WWX:C17	2.32	0.43
1:C:167:TYR:CD1	1:C:234:MET:HA	2.54	0.42
1:C:8:GLY:O	1:C:11:GLY:HA3	2.19	0.42
1:B:127:PRO:HG2	1:B:128:ASP:OD1	2.19	0.42
1:C:167:TYR:CD2	1:C:234:MET:CG	3.03	0.42
1:B:252[A]:PHE:CZ	1:B:255[A]:ARG:CB	3.02	0.42
1:A:103:SER:O	1:A:111:HIS:CD2	2.71	0.42
1:A:192:ARG:HD2	1:A:207:LEU:HD11	2.02	0.42
1:D:52:ASN:HA	1:D:178:ASN:HA	2.01	0.42
1:D:61:LEU:O	1:D:171:GLU:HA	2.20	0.41
1:A:7:PHE:HE2	1:A:240:ARG:HH11	1.66	0.41
1:C:119:VAL:HG11	4:C:303:WWX:F12	2.10	0.41
1:A:253:ASP:OD2	5:A:487:HOH:O	2.21	0.41
1:C:114:ALA:HB3	1:C:146:ILE:HB	2.02	0.41
1:C:61:LEU:HG	1:C:70:LEU:CD1	2.51	0.40
1:C:63[B]:ASN:OD1	1:C:165:VAL:O	2.40	0.40
1:A:174:VAL:HA	1:A:175:PRO:HD3	1.98	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	264/263 (100%)	261 (99%)	3 (1%)	0	100	100
1	B	265/263 (101%)	258 (97%)	7 (3%)	0	100	100
1	C	266/263 (101%)	253 (95%)	13 (5%)	0	100	100
1	D	267/263 (102%)	258 (97%)	9 (3%)	0	100	100
All	All	1062/1052 (101%)	1030 (97%)	32 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	238/235 (101%)	232 (98%)	6 (2%)	53	20
1	B	239/235 (102%)	230 (96%)	9 (4%)	38	7
1	C	240/235 (102%)	228 (95%)	12 (5%)	28	4
1	D	241/235 (103%)	234 (97%)	7 (3%)	48	15
All	All	958/940 (102%)	924 (96%)	34 (4%)	44	10

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	LYS
1	A	42	SER

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Mol	Chain	Res	Type
1	A	82	GLN
1	A	136	SER
1	A	156	ASP
1	A	163	GLN
1	B	49	GLN
1	B	89	GLN
1	B	130[A]	SER
1	B	130[B]	SER
1	B	156	ASP
1	B	219[A]	GLN
1	B	219[B]	GLN
1	B	252[A]	PHE
1	B	252[B]	PHE
1	C	61	LEU
1	C	73	PRO
1	C	75	ASP
1	C	92	LEU
1	C	128	ASP
1	C	130	SER
1	C	154	SER
1	C	156	ASP
1	C	162	LEU
1	C	219	GLN
1	C	234	MET
1	C	235	ASP
1	D	3	LYS
1	D	20	PRO
1	D	49	GLN
1	D	89[A]	GLN
1	D	89[B]	GLN
1	D	156	ASP
1	D	192	ARG

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

Mol	Chain	Res	Type
1	A	33	HIS
1	A	49	GLN
1	A	58	GLN
1	A	66	HIS
1	A	82	GLN
1	A	110	GLN

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Mol	Chain	Res	Type
1	A	164	HIS
1	B	49	GLN
1	B	77	HIS
1	B	82	GLN
1	B	101	HIS
1	B	111	HIS
1	C	49	GLN
1	C	111	HIS
1	C	219	GLN
1	C	233	HIS
1	D	49	GLN
1	D	164	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 15 ligands modelled in this entry, 4 are monoatomic - leaving 11 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	EDO	A	302	-	3,3,3	0.71	0	2,2,2	0.16	0
4	WWX	A	303	2	36,37,37	2.51	11 (30%)	47,55,55	3.52	19 (40%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	EDO	B	302	-	3,3,3	0.87	0	2,2,2	0.26	0
4	WWX	B	303	2	36,37,37	2.96	12 (33%)	47,55,55	4.46	27 (57%)
3	EDO	C	302	-	3,3,3	0.31	0	2,2,2	0.79	0
4	WWX	C	303	2	36,37,37	2.87	16 (44%)	47,55,55	2.92	14 (29%)
3	EDO	D	302	-	3,3,3	0.46	0	2,2,2	0.37	0
3	EDO	D	303	-	3,3,3	0.54	0	2,2,2	0.37	0
3	EDO	D	304	-	3,3,3	0.99	0	2,2,2	0.75	0
4	WWX	D	305[A]	2	36,37,37	2.12	7 (19%)	47,55,55	2.39	10 (21%)
4	WWX	D	305[B]	2	36,37,37	2.15	7 (19%)	47,55,55	2.31	12 (25%)

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	EDO	A	302	-	-	0/1/1/1	0/0/0/0
4	WWX	A	303	2	-	0/32/32/32	0/3/3/3
3	EDO	B	302	-	-	0/1/1/1	0/0/0/0
4	WWX	B	303	2	-	0/32/32/32	0/3/3/3
3	EDO	C	302	-	-	0/1/1/1	0/0/0/0
4	WWX	C	303	2	-	0/32/32/32	0/3/3/3
3	EDO	D	302	-	-	0/1/1/1	0/0/0/0
3	EDO	D	303	-	-	0/1/1/1	0/0/0/0
3	EDO	D	304	-	-	0/1/1/1	0/0/0/0
4	WWX	D	305[A]	2	-	0/32/32/32	0/3/3/3
4	WWX	D	305[B]	2	-	0/32/32/32	0/3/3/3

All (53) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	303	WWX	C23-C22	-2.64	1.47	1.51
4	A	303	WWX	O29-C22	-2.52	1.37	1.42
4	B	303	WWX	C35-C30	-2.26	1.35	1.39
4	A	303	WWX	F13-C10	-2.18	1.31	1.35
4	A	303	WWX	C6-C5	-2.14	1.37	1.39
4	C	303	WWX	C35-C30	2.01	1.42	1.39
4	D	305[A]	WWX	C25-C24	2.12	1.42	1.38
4	A	303	WWX	C28-C23	2.13	1.42	1.39
4	A	303	WWX	C21-N19	2.17	1.49	1.46
4	D	305[B]	WWX	C25-C24	2.17	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	305[B]	WWX	C17-S14	2.28	1.83	1.78
4	C	303	WWX	C34-C35	2.29	1.43	1.38
4	D	305[A]	WWX	C17-S14	2.45	1.83	1.78
4	B	303	WWX	F11-C6	2.47	1.39	1.35
4	C	303	WWX	C5-S1	2.66	1.83	1.79
4	B	303	WWX	O3-S1	2.67	1.49	1.43
4	C	303	WWX	C31-C30	2.73	1.43	1.39
4	C	303	WWX	F11-C6	2.83	1.39	1.35
4	A	303	WWX	C26-C25	2.84	1.44	1.38
4	A	303	WWX	C34-C35	2.91	1.44	1.38
4	C	303	WWX	C9-C10	3.00	1.43	1.39
4	B	303	WWX	C24-C23	3.11	1.44	1.39
4	C	303	WWX	C21-C22	3.13	1.60	1.54
4	B	303	WWX	C6-C5	3.23	1.43	1.39
4	C	303	WWX	C28-C23	3.31	1.44	1.39
4	B	303	WWX	C31-C30	3.31	1.44	1.39
4	C	303	WWX	C26-C25	3.39	1.46	1.38
4	D	305[A]	WWX	O3-S1	3.43	1.50	1.43
4	D	305[B]	WWX	O3-S1	3.48	1.51	1.43
4	C	303	WWX	O2-S1	3.53	1.51	1.43
4	C	303	WWX	O3-S1	3.59	1.51	1.43
4	C	303	WWX	C9-C8	3.59	1.44	1.40
4	B	303	WWX	C9-C10	3.81	1.44	1.39
4	C	303	WWX	O15-S14	4.06	1.50	1.44
4	D	305[B]	WWX	O2-S1	4.15	1.52	1.43
4	D	305[A]	WWX	O2-S1	4.17	1.52	1.43
4	A	303	WWX	O3-S1	4.48	1.53	1.43
4	D	305[B]	WWX	S1-N4	4.56	1.70	1.60
4	D	305[A]	WWX	S1-N4	4.56	1.70	1.60
4	B	303	WWX	F12-C7	4.59	1.42	1.35
4	A	303	WWX	O2-S1	4.76	1.53	1.43
4	B	303	WWX	S1-N4	5.72	1.72	1.60
4	D	305[A]	WWX	O15-S14	5.84	1.53	1.44
4	D	305[B]	WWX	O15-S14	6.04	1.53	1.44
4	D	305[A]	WWX	O16-S14	6.61	1.54	1.44
4	B	303	WWX	C5-S1	6.69	1.90	1.79
4	D	305[B]	WWX	O16-S14	6.78	1.54	1.44
4	A	303	WWX	O16-S14	7.24	1.55	1.44
4	B	303	WWX	O15-S14	7.56	1.56	1.44
4	B	303	WWX	O16-S14	7.81	1.56	1.44
4	A	303	WWX	O15-S14	7.94	1.56	1.44
4	C	303	WWX	S1-N4	8.07	1.77	1.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	303	WWX	O16-S14	8.59	1.57	1.44

All (82) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	303	WWX	O16-S14-O15	-15.35	99.07	118.42
4	A	303	WWX	O16-S14-O15	-12.87	102.20	118.42
4	C	303	WWX	O16-S14-O15	-11.58	103.82	118.42
4	D	305[A]	WWX	O16-S14-O15	-11.36	104.11	118.42
4	D	305[B]	WWX	O16-S14-O15	-10.41	105.31	118.42
4	B	303	WWX	C5-S1-N4	-7.64	93.54	108.24
4	B	303	WWX	C6-C7-C8	-7.56	113.50	121.68
4	A	303	WWX	C25-C24-C23	-6.58	112.56	120.64
4	A	303	WWX	O2-S1-O3	-6.49	106.79	118.70
4	B	303	WWX	O2-S1-O3	-5.76	108.13	118.70
4	B	303	WWX	F11-C6-C7	-5.35	108.34	119.29
4	A	303	WWX	C30-C21-N19	-5.12	107.04	113.61
4	B	303	WWX	F13-C10-C5	-5.00	111.45	120.54
4	B	303	WWX	O2-S1-N4	-4.86	99.70	107.34
4	C	303	WWX	O2-S1-O3	-4.72	110.04	118.70
4	B	303	WWX	C7-C8-S14	-4.67	109.21	120.53
4	A	303	WWX	O2-S1-C5	-4.63	100.49	107.36
4	B	303	WWX	C28-C23-C22	-4.44	114.23	120.73
4	B	303	WWX	O16-S14-C8	-4.43	95.15	106.54
4	D	305[A]	WWX	O2-S1-C5	-4.23	101.08	107.36
4	D	305[B]	WWX	O2-S1-C5	-4.23	101.09	107.36
4	C	303	WWX	O15-S14-C8	-3.92	96.46	106.54
4	C	303	WWX	O2-S1-C5	-3.82	101.70	107.36
4	A	303	WWX	C24-C23-C22	-3.60	115.45	120.73
4	A	303	WWX	O15-S14-C17	-3.52	102.39	108.18
4	A	303	WWX	F13-C10-C5	-3.49	114.19	120.54
4	D	305[A]	WWX	C25-C24-C23	-3.46	116.39	120.64
4	D	305[B]	WWX	C25-C24-C23	-3.44	116.41	120.64
4	B	303	WWX	C31-C30-C21	-3.34	115.51	120.79
4	D	305[A]	WWX	C30-C21-N19	-3.29	109.39	113.61
4	D	305[B]	WWX	C30-C21-N19	-3.11	109.61	113.61
4	D	305[A]	WWX	O2-S1-O3	-3.00	113.20	118.70
4	D	305[B]	WWX	O2-S1-O3	-2.99	113.22	118.70
4	C	303	WWX	C28-C23-C22	-2.99	116.35	120.73
4	A	303	WWX	C26-C27-C28	-2.97	116.13	120.21
4	A	303	WWX	C7-C8-S14	-2.97	113.34	120.53
4	A	303	WWX	O20-C18-C17	-2.91	104.53	110.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	303	WWX	C34-C33-C32	-2.81	115.21	119.89
4	B	303	WWX	O20-C18-C17	-2.63	105.09	110.38
4	D	305[A]	WWX	O20-C18-C17	-2.55	105.25	110.38
4	A	303	WWX	C6-C7-C8	-2.53	118.95	121.68
4	C	303	WWX	C27-C28-C23	-2.48	117.59	120.64
4	B	303	WWX	C25-C24-C23	-2.47	117.60	120.64
4	B	303	WWX	C32-C31-C30	-2.28	117.84	120.64
4	D	305[B]	WWX	C28-C23-C22	-2.21	117.50	120.73
4	D	305[B]	WWX	O20-C18-C17	-2.20	105.95	110.38
4	D	305[A]	WWX	C28-C23-C22	-2.19	117.52	120.73
4	B	303	WWX	C28-C23-C24	2.05	120.88	118.30
4	C	303	WWX	C6-C7-C8	2.10	123.96	121.68
4	D	305[B]	WWX	O16-S14-C17	2.13	111.69	108.18
4	D	305[A]	WWX	C28-C23-C24	2.20	121.06	118.30
4	D	305[B]	WWX	C28-C23-C24	2.24	121.11	118.30
4	D	305[B]	WWX	O16-S14-C8	2.28	112.41	106.54
4	A	303	WWX	C26-C25-C24	2.45	123.58	120.21
4	B	303	WWX	C10-C9-C8	2.49	120.36	116.06
4	C	303	WWX	C10-C9-C8	2.50	120.38	116.06
4	B	303	WWX	C30-C21-C22	2.55	119.24	111.73
4	D	305[A]	WWX	C10-C5-C6	2.70	118.46	116.58
4	C	303	WWX	C28-C23-C24	2.72	121.71	118.30
4	A	303	WWX	O16-S14-C17	2.80	112.79	108.18
4	B	303	WWX	C24-C23-C22	2.83	124.87	120.73
4	A	303	WWX	O16-S14-C8	2.92	114.04	106.54
4	D	305[B]	WWX	C10-C5-C6	2.99	118.66	116.58
4	B	303	WWX	C17-S14-C8	3.02	121.57	109.39
4	B	303	WWX	O3-S1-N4	3.15	112.29	107.34
4	B	303	WWX	C35-C30-C31	3.38	122.54	118.30
4	C	303	WWX	O29-C22-C23	3.49	118.84	111.18
4	B	303	WWX	O29-C22-C21	3.51	115.90	107.34
4	B	303	WWX	O2-S1-C5	3.82	113.03	107.36
4	C	303	WWX	C33-C32-C31	4.26	126.06	120.21
4	A	303	WWX	F13-C10-C9	4.39	125.81	119.49
4	B	303	WWX	C7-C6-C5	5.22	127.33	121.68
4	A	303	WWX	C28-C23-C24	5.63	125.36	118.30
4	D	305[B]	WWX	C5-S1-N4	5.86	119.52	108.24
4	D	305[A]	WWX	C5-S1-N4	5.88	119.56	108.24
4	B	303	WWX	O15-S14-C17	5.94	117.96	108.18
4	A	303	WWX	C10-C5-C6	6.72	121.25	116.58
4	C	303	WWX	O15-S14-C17	7.04	119.77	108.18
4	B	303	WWX	F13-C10-C9	7.25	129.92	119.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	303	WWX	C5-S1-N4	7.86	123.36	108.24
4	A	303	WWX	C5-S1-N4	8.44	124.48	108.24
4	B	303	WWX	O3-S1-C5	12.66	126.16	107.36

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	303	WWX	5	0
4	C	303	WWX	1	0
3	D	302	EDO	3	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	260/263 (98%)	-0.20	3 (1%) 79 83	7, 17, 34, 47	0
1	B	261/263 (99%)	-0.15	5 (1%) 67 73	7, 13, 39, 52	0
1	C	260/263 (98%)	0.37	22 (8%) 11 13	9, 21, 41, 65	0
1	D	260/263 (98%)	-0.35	1 (0%) 92 94	8, 13, 25, 37	0
All	All	1041/1052 (98%)	-0.08	31 (2%) 51 59	7, 15, 35, 65	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	252[A]	PHE	5.2
1	C	61	LEU	4.9
1	C	55	ALA	4.1
1	C	9	PRO	4.1
1	C	3	LYS	4.1
1	C	8	GLY	3.2
1	C	165	VAL	3.2
1	C	177	PHE	3.1
1	C	179	ILE	3.0
1	C	56	ASN	3.0
1	C	173	PHE	3.0
1	C	235	ASP	2.8
1	C	167	TYR	2.6
1	C	10	ASP	2.5
1	C	70	LEU	2.5
1	B	137	GLU	2.5
1	C	174	VAL	2.5
1	C	169	GLY	2.5
1	A	7	PHE	2.4
1	C	230[A]	TYR	2.4
1	A	82	GLN	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	171	GLU	2.3
1	C	58	GLN	2.3
1	C	51	TYR	2.2
1	B	136	SER	2.2
1	B	253	ASP	2.1
1	A	8	GLY	2.1
1	C	59	PHE	2.1
1	D	252	PHE	2.1
1	B	164	HIS	2.0
1	C	158	ILE	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
3	EDO	D	302	4/4	0.92	0.17	8.27	28,32,33,36	0
4	WWX	B	303	35/35	0.91	0.19	8.11	14,31,44,47	0
4	WWX	A	303	35/35	0.94	0.14	5.47	12,22,29,38	0
3	EDO	D	304	4/4	0.84	0.10	3.42	26,28,28,33	0
4	WWX	D	305[A]	35/35	0.96	0.13	3.05	11,17,19,20	35
4	WWX	D	305[B]	35/35	0.96	0.13	3.05	11,17,19,23	35
3	EDO	A	302	4/4	0.93	0.10	1.83	30,32,33,34	0
4	WWX	C	303	35/35	0.94	0.13	1.76	10,21,26,33	0
3	EDO	B	302	4/4	0.82	0.10	0.59	25,26,33,35	0
3	EDO	D	303	4/4	0.91	0.16	-	35,39,40,43	0
2	ZN	B	301	1/1	1.00	0.05	-	8,8,8,8	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	ZN	A	301	1/1	1.00	0.06	-	9,9,9,9	0
3	EDO	C	302	4/4	0.87	0.12	-	33,38,38,41	0
2	ZN	C	301	1/1	0.99	0.07	-	14,14,14,14	0
2	ZN	D	301	1/1	1.00	0.07	-	8,8,8,8	0

6.5 Other polymers [i](#)

There are no such residues in this entry.