Full wwPDB X-ray Structure Validation Report ⓘ

May 21, 2020 – 04:25 am BST

PDB ID	:	5OYN
Title	:	Crystal structure of D-xylonate dehydratase in holo-form
Authors	:	Rahman, M.M.; Rouvinen, J.; Hakulinen, N.
Deposited on	:	2017-09-11
Resolution	:	2.70 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 ⓘ symbol.

The following versions of software and data (see references ⓘ) were used in the production of this report:

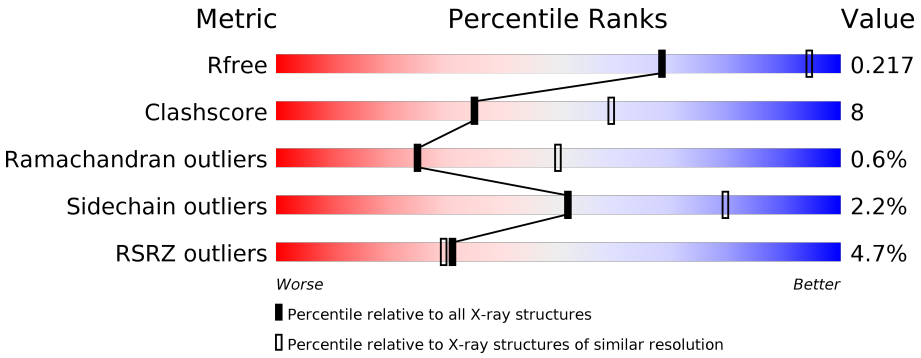
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 2.70 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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 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 <=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	600	6% 80% 18%
1	B	600	9% 71% 27%
1	C	600	2% 79% 18%
1	D	600	2% 85% 13%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 18336 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 Dehydratase, IlvD/Edd family.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	589	Total	C	N	O	S	0	0	0
			4502	2820	808	852	22			
1	B	589	Total	C	N	O	S	0	0	0
			4502	2820	808	852	22			
1	C	588	Total	C	N	O	S	0	0	0
			4494	2816	806	850	22			
1	D	588	Total	C	N	O	S	0	0	0
			4494	2816	806	850	22			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-8	MET	-	initiating methionine	UNP Q9A9Z2
A	-7	ASP	-	expression tag	UNP Q9A9Z2
A	-6	TRP	-	expression tag	UNP Q9A9Z2
A	-5	SER	-	expression tag	UNP Q9A9Z2
A	-4	HIS	-	expression tag	UNP Q9A9Z2
A	-3	PRO	-	expression tag	UNP Q9A9Z2
A	-2	GLN	-	expression tag	UNP Q9A9Z2
A	-1	PHE	-	expression tag	UNP Q9A9Z2
A	0	GLU	-	expression tag	UNP Q9A9Z2
A	1	LYS	-	expression tag	UNP Q9A9Z2
B	-8	MET	-	initiating methionine	UNP Q9A9Z2
B	-7	ASP	-	expression tag	UNP Q9A9Z2
B	-6	TRP	-	expression tag	UNP Q9A9Z2
B	-5	SER	-	expression tag	UNP Q9A9Z2
B	-4	HIS	-	expression tag	UNP Q9A9Z2
B	-3	PRO	-	expression tag	UNP Q9A9Z2
B	-2	GLN	-	expression tag	UNP Q9A9Z2
B	-1	PHE	-	expression tag	UNP Q9A9Z2
B	0	GLU	-	expression tag	UNP Q9A9Z2
B	1	LYS	-	expression tag	UNP Q9A9Z2
C	-8	MET	-	initiating methionine	UNP Q9A9Z2

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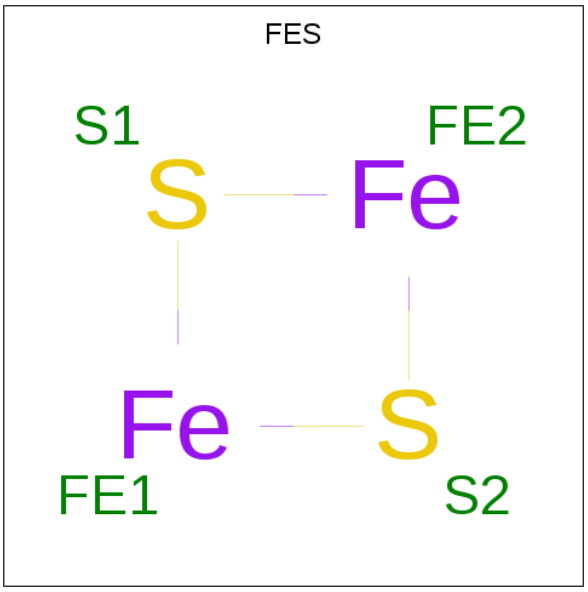
Chain	Residue	Modelled	Actual	Comment	Reference
C	-7	ASP	-	expression tag	UNP Q9A9Z2
C	-6	TRP	-	expression tag	UNP Q9A9Z2
C	-5	SER	-	expression tag	UNP Q9A9Z2
C	-4	HIS	-	expression tag	UNP Q9A9Z2
C	-3	PRO	-	expression tag	UNP Q9A9Z2
C	-2	GLN	-	expression tag	UNP Q9A9Z2
C	-1	PHE	-	expression tag	UNP Q9A9Z2
C	0	GLU	-	expression tag	UNP Q9A9Z2
C	1	LYS	-	expression tag	UNP Q9A9Z2
D	-8	MET	-	initiating methionine	UNP Q9A9Z2
D	-7	ASP	-	expression tag	UNP Q9A9Z2
D	-6	TRP	-	expression tag	UNP Q9A9Z2
D	-5	SER	-	expression tag	UNP Q9A9Z2
D	-4	HIS	-	expression tag	UNP Q9A9Z2
D	-3	PRO	-	expression tag	UNP Q9A9Z2
D	-2	GLN	-	expression tag	UNP Q9A9Z2
D	-1	PHE	-	expression tag	UNP Q9A9Z2
D	0	GLU	-	expression tag	UNP Q9A9Z2
D	1	LYS	-	expression tag	UNP Q9A9Z2

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 3 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).



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

- Molecule 4 is water.

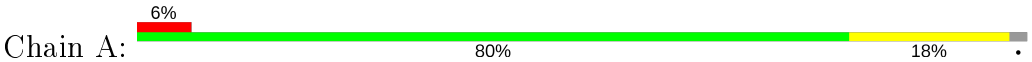
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	74	Total O 74 74	0	0
4	B	49	Total O 49 49	0	0
4	C	92	Total O 92 92	0	0
4	D	109	Total O 109 109	0	0

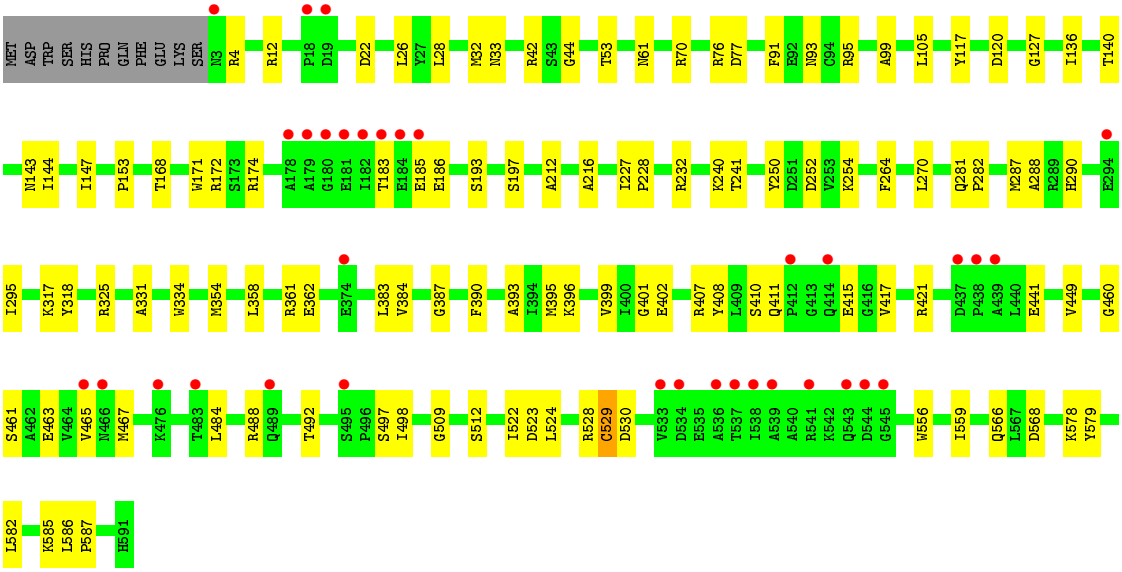
3 Residue-property plots (i)

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: Dehydratase, IlvD/Edd family

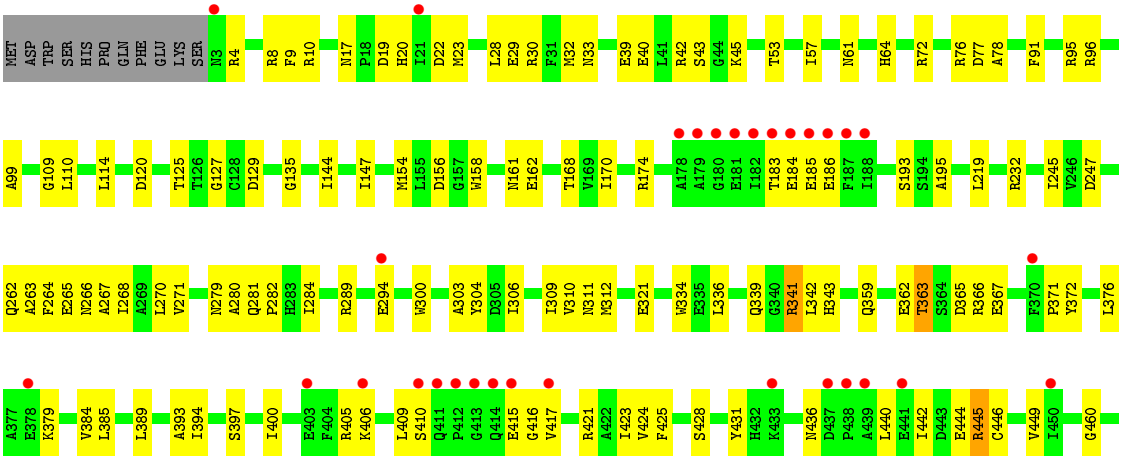
Chain A:

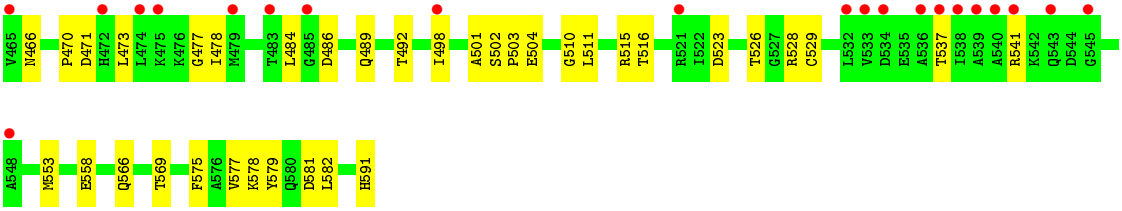




- Molecule 1: Dehydratase, IlvD/Edd family

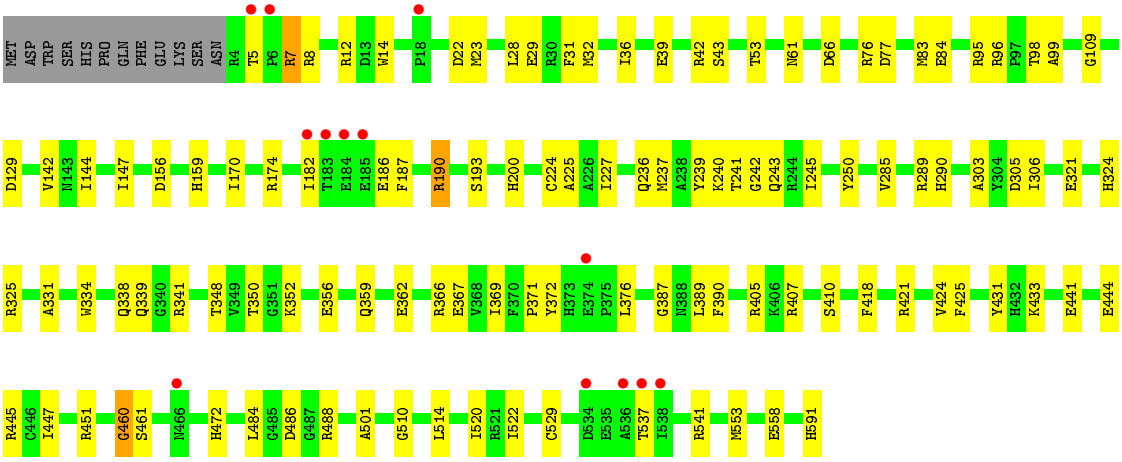
Chain B:





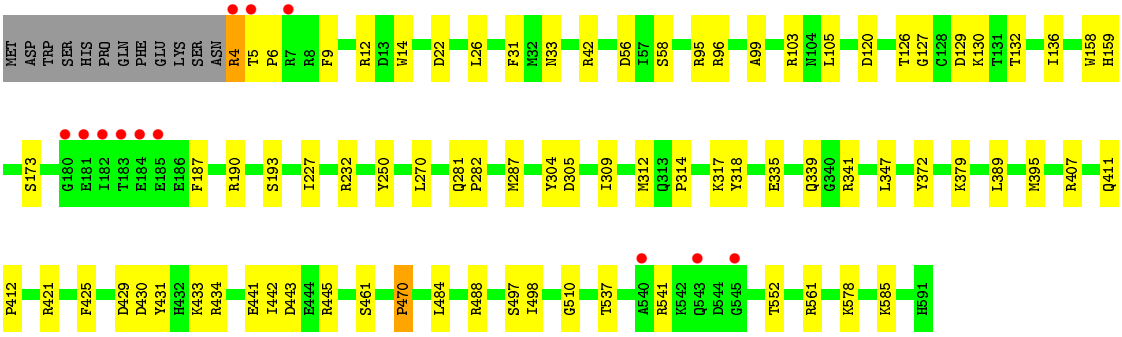
• Molecule 1: Dehydratase, IlvD/Edd family

Chain C:



• Molecule 1: Dehydratase, IlvD/Edd family

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	270.42Å 236.13Å 65.16Å 90.00° 97.38° 90.00°	Depositor
Resolution (Å)	29.93 – 2.70 29.94 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.6 (29.93-2.70) 99.6 (29.94-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.61 (at 2.68Å)	Xtriage
Refinement program	PHENIX (1.12_2829: ???)	Depositor
R, R_{free}	0.177 , 0.217 0.177 , 0.217	Depositor DCC
R_{free} test set	5512 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	66.2	Xtriage
Anisotropy	0.497	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 49.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	18336	wwPDB-VP
Average B, all atoms (Å^2)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.65% 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

5.1 Standard geometry

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

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	0.39	0/4586	0.58	2/6229 (0.0%)
1	B	0.36	0/4586	0.57	0/6229
1	C	0.40	0/4578	0.57	0/6218
1	D	0.42	0/4578	0.59	0/6218
All	All	0.39	0/18328	0.58	2/24894 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	28	LEU	CA-CB-CG	6.84	131.03	115.30
1	A	410	SER	C-N-CA	-5.28	108.51	121.70

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	4502	0	4442	81	0
1	B	4502	0	4443	119	0
1	C	4494	0	4437	70	0
1	D	4494	0	4436	48	0
2	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	0	0	0
3	B	4	0	0	0	0
3	C	4	0	0	1	0
3	D	4	0	0	0	0
4	A	74	0	0	3	0
4	B	49	0	0	1	0
4	C	92	0	0	6	0
4	D	109	0	0	1	0
All	All	18336	0	17758	292	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 8.

All (292) 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:528:ARG:NH1	1:A:530:ASP:OD2	1.64	1.28
1:B:473:LEU:HB3	1:B:478:ILE:HD11	1.28	1.13
1:A:528:ARG:HH12	1:A:530:ASP:CG	1.64	0.99
1:B:409:LEU:C	1:B:409:LEU:HD13	1.92	0.89
1:B:409:LEU:HD21	1:B:416:GLY:H	1.41	0.85
1:B:442:ILE:HG21	1:B:470:PRO:HG2	1.61	0.82
1:B:484:LEU:HD12	1:B:498:ILE:HB	1.62	0.82
1:B:409:LEU:CD2	1:B:416:GLY:H	1.95	0.79
1:B:363:THR:HG22	1:B:365:ASP:H	1.49	0.78
1:B:473:LEU:HB3	1:B:478:ILE:CD1	2.14	0.75
1:C:5:THR:HG23	1:C:7:ARG:HH12	1.51	0.75
1:B:515:ARG:HB2	1:B:515:ARG:NH1	2.02	0.74
1:B:29:GLU:OE2	1:B:30:ARG:NE	2.16	0.74
1:B:409:LEU:HD21	1:B:415:GLU:HA	1.68	0.73
1:A:240:LYS:NZ	4:A:701:HOH:O	2.20	0.73
1:B:449:VAL:HG22	1:B:484:LEU:HB3	1.71	0.72
1:B:168:THR:HG22	1:B:492:THR:O	1.89	0.72
1:B:409:LEU:HD13	1:B:409:LEU:O	1.90	0.70
1:B:397:SER:O	1:B:400:ILE:HG13	1.93	0.68
1:B:400:ILE:HD13	1:B:405:ARG:NH1	2.08	0.67
1:B:310:VAL:HG12	1:B:312:MET:HB2	1.76	0.66
1:A:136:ILE:O	1:A:140:THR:HG23	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:183:THR:HG23	1:B:186:GLU:H	1.62	0.65
1:C:224:CYS:HB2	1:C:237:MET:SD	2.35	0.65
1:B:28:LEU:HD11	1:B:42:ARG:HD3	1.78	0.65
1:B:423:ILE:HD11	1:B:446:CYS:SG	2.37	0.65
1:C:366:ARG:HD2	1:C:371:PRO:HD3	1.79	0.64
1:D:347:LEU:H	1:D:347:LEU:HD23	1.63	0.64
1:A:183:THR:HG22	1:A:186:GLU:HG3	1.79	0.64
1:C:7:ARG:NE	1:C:250:TYR:O	2.32	0.63
1:A:566:GLN:HB2	1:A:568:ASP:OD1	1.99	0.63
1:D:389:LEU:HA	1:D:510:GLY:HA3	1.81	0.62
1:A:407:ARG:HD2	1:A:408:TYR:CZ	2.34	0.62
1:B:339:GLN:HG3	1:B:372:TYR:CD2	2.35	0.62
1:C:23:MET:HE1	1:C:591:HIS:HB2	1.80	0.62
1:B:4:ARG:NH1	1:B:78:ALA:O	2.32	0.61
1:B:537:THR:O	1:B:541:ARG:HG3	2.01	0.61
1:A:174:ARG:NH1	1:B:22:ASP:OD2	2.34	0.60
1:B:478:ILE:O	1:B:478:ILE:HD12	2.02	0.60
1:D:442:ILE:HD12	1:D:470:PRO:HG3	1.82	0.60
1:D:421:ARG:NH2	1:D:441:GLU:O	2.34	0.60
1:B:162:GLU:OE2	1:B:162:GLU:N	2.35	0.60
1:B:409:LEU:HD21	1:B:416:GLY:N	2.15	0.60
1:B:32:MET:O	1:D:232:ARG:HG3	2.01	0.60
1:A:395:MET:HG3	1:A:498:ILE:HG13	1.84	0.60
1:B:264:PHE:O	1:B:268:ILE:HG13	2.02	0.59
1:D:429:ASP:OD1	1:D:433:LYS:HE2	2.03	0.59
1:B:4:ARG:NH2	1:B:247:ASP:OD1	2.36	0.59
1:A:91:PHE:CE1	1:A:93:ASN:HB2	2.38	0.59
1:B:409:LEU:C	1:B:409:LEU:CD1	2.67	0.59
1:C:407:ARG:HD3	1:C:444:GLU:HG3	1.84	0.59
1:B:575:PHE:O	1:B:578:LYS:HE3	2.03	0.58
1:B:400:ILE:HD13	1:B:405:ARG:HH11	1.69	0.58
1:D:305:ASP:OD1	1:D:341:ARG:NH2	2.35	0.58
1:A:579:TYR:HB3	1:A:582:LEU:HD21	1.84	0.58
1:B:417:VAL:HG22	1:B:523:ASP:OD2	2.04	0.57
1:C:305:ASP:OD2	1:C:341:ARG:NH2	2.32	0.57
1:B:409:LEU:O	1:B:409:LEU:CD1	2.52	0.57
1:A:390:PHE:HE2	1:A:484:LEU:HD11	1.70	0.57
1:C:159:HIS:CD2	1:C:190:ARG:HG3	2.40	0.57
1:B:470:PRO:HD2	1:B:473:LEU:HD12	1.86	0.56
1:B:515:ARG:CB	1:B:515:ARG:NH1	2.68	0.56
1:C:77:ASP:OD2	1:C:239:TYR:OH	2.20	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:486:ASP:HA	1:C:501:ALA:HB3	1.86	0.56
1:C:334:TRP:CZ2	1:C:362:GLU:HB2	2.41	0.56
1:D:585:LYS:HD3	1:D:585:LYS:O	2.05	0.56
1:B:64:HIS:CD2	1:B:125:THR:HB	2.40	0.56
1:D:304:TYR:CE2	1:D:379:LYS:HD3	2.41	0.55
1:B:311:ASN:HA	1:B:376:LEU:HD11	1.88	0.55
1:B:366:ARG:HD2	1:B:371:PRO:HD3	1.89	0.54
1:D:95:ARG:HG2	1:D:99:ALA:HA	1.88	0.54
1:A:264:PHE:HB3	1:A:295:ILE:HD11	1.88	0.54
1:D:9:PHE:HB3	1:D:120:ASP:OD1	2.08	0.54
1:C:96:ARG:HD3	1:D:14:TRP:CZ2	2.43	0.54
1:A:396:LYS:HE2	1:A:399:VAL:HG21	1.89	0.54
1:D:103:ARG:HB2	1:D:130:KCX:HG3	1.90	0.54
1:A:585:LYS:HB3	1:B:553:MET:HE3	1.88	0.53
1:C:367:GLU:OE1	4:C:701:HOH:O	2.18	0.53
1:A:463:GLU:OE1	1:B:591:HIS:NE2	2.41	0.53
1:D:430:ASP:OD1	1:D:434:ARG:HD3	2.09	0.53
1:D:430:ASP:OD2	1:D:434:ARG:NH1	2.41	0.53
1:B:336:LEU:HB2	1:B:342:LEU:HG	1.91	0.53
1:B:515:ARG:HH11	1:B:515:ARG:CB	2.22	0.53
1:C:421:ARG:NH2	1:C:441:GLU:O	2.41	0.53
1:B:267:ALA:O	1:B:271:VAL:HG23	2.08	0.53
1:B:421:ARG:NH2	1:B:440:LEU:O	2.42	0.53
1:D:12:ARG:N	1:D:12:ARG:HD2	2.24	0.53
1:A:334:TRP:CZ3	1:A:362:GLU:HG3	2.44	0.52
1:A:95:ARG:HG2	1:A:99:ALA:HA	1.92	0.52
1:C:147:ILE:HD13	1:C:241:THR:HG23	1.89	0.52
1:A:168:THR:HG22	1:A:492:THR:O	2.09	0.52
1:A:317:LYS:HD3	1:A:318:TYR:CZ	2.44	0.52
1:B:425:PHE:CD2	1:B:431:TYR:HA	2.44	0.52
1:B:262:GLN:HG2	1:B:343:HIS:CD2	2.45	0.51
1:C:331:ALA:HB3	1:C:369:ILE:HD13	1.92	0.51
1:A:216:ALA:HB2	1:A:270:LEU:HD22	1.92	0.51
1:C:334:TRP:O	1:C:338:GLN:HG2	2.10	0.51
1:D:339:GLN:HG3	1:D:372:TYR:CG	2.44	0.51
1:A:461:SER:O	1:A:488:ARG:NH1	2.44	0.51
1:C:405:ARG:HD2	4:C:721:HOH:O	2.10	0.51
1:C:5:THR:HG23	1:C:7:ARG:NH1	2.22	0.51
1:C:109:GLY:HA2	1:D:105:LEU:HD21	1.93	0.51
1:A:117:TYR:HE2	1:B:91:PHE:HB3	1.76	0.51
1:A:415:GLU:OE1	1:A:415:GLU:N	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:461:SER:O	1:D:488:ARG:NH1	2.43	0.51
1:B:303:ALA:HA	1:B:306:ILE:HD13	1.93	0.50
1:A:212:ALA:HB1	1:A:270:LEU:HD21	1.94	0.50
1:A:587:PRO:O	1:B:96:ARG:NH2	2.41	0.50
1:C:142:VAL:HG12	1:C:144:ILE:HG23	1.92	0.50
1:A:384:VAL:HA	1:A:393:ALA:O	2.12	0.50
1:B:473:LEU:CB	1:B:478:ILE:HD11	2.19	0.50
1:D:407:ARG:O	1:D:445:ARG:NH1	2.45	0.50
1:B:265:GLU:OE1	1:B:343:HIS:NE2	2.28	0.50
1:C:558:GLU:OE2	1:D:578:LYS:NZ	2.45	0.49
1:A:461:SER:HB2	1:A:488:ARG:HG3	1.94	0.49
1:B:183:THR:OG1	1:B:184:GLU:N	2.45	0.49
1:D:4:ARG:HD2	1:D:250:TYR:CE2	2.48	0.49
1:A:53:THR:HB	1:A:61:ASN:HD22	1.77	0.49
1:B:515:ARG:HB2	1:B:515:ARG:CZ	2.42	0.49
1:A:559:ILE:HD11	1:B:575:PHE:HZ	1.78	0.49
1:C:240:LYS:NZ	1:C:243:GLN:OE1	2.46	0.49
1:A:252:ASP:OD1	1:A:254:LYS:NZ	2.46	0.49
1:C:418:PHE:CZ	1:C:522:ILE:HD12	2.48	0.49
1:C:421:ARG:NH1	4:C:705:HOH:O	2.35	0.49
1:C:285:VAL:O	1:C:289:ARG:HG3	2.13	0.48
1:C:348:THR:OG1	1:C:350:THR:OG1	2.27	0.48
1:C:242:GLY:O	1:C:245:ILE:HG22	2.13	0.48
1:A:76:ARG:HG2	1:C:77:ASP:OD1	2.13	0.48
1:D:173:SER:OG	1:D:190:ARG:NH2	2.45	0.48
1:D:281:GLN:HB3	1:D:282:PRO:HD3	1.95	0.48
1:B:304:TYR:CE2	1:B:379:LYS:HD3	2.49	0.48
1:C:156:ASP:OD1	1:C:321:GLU:HB2	2.14	0.48
1:A:387:GLY:HA2	1:A:528:ARG:NH2	2.29	0.48
1:B:384:VAL:O	1:B:385:LEU:HD23	2.13	0.48
1:B:23:MET:HE1	1:B:591:HIS:HB2	1.96	0.48
1:C:227:ILE:HG12	1:C:324:HIS:CE1	2.49	0.48
1:D:12:ARG:HH22	1:D:42:ARG:HA	1.79	0.48
1:C:290:HIS:HE1	4:C:759:HOH:O	1.97	0.48
1:B:183:THR:HG23	1:B:185:GLU:H	1.79	0.47
1:A:22:ASP:OD2	1:B:174:ARG:HD3	2.14	0.47
1:B:436:ASN:HD21	1:B:471:ASP:CG	2.18	0.47
1:B:423:ILE:HA	1:B:516:THR:HG23	1.95	0.47
1:B:72:ARG:O	1:B:76:ARG:HG3	2.13	0.47
1:A:77:ASP:OD1	1:C:76:ARG:HD3	2.15	0.47
1:B:304:TYR:CZ	1:B:379:LYS:HD3	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:553:MET:HE3	4:C:787:HOH:O	2.13	0.47
1:B:183:THR:HG22	1:B:186:GLU:OE1	2.15	0.47
1:C:39:GLU:O	1:C:43:SER:HB3	2.15	0.47
1:B:147:ILE:HG22	1:B:245:ILE:HD13	1.97	0.47
1:B:183:THR:CG2	1:B:186:GLU:H	2.27	0.47
1:B:504:GLU:HG2	1:B:566:GLN:OE1	2.15	0.47
1:B:45:LYS:NZ	4:B:701:HOH:O	2.31	0.47
1:C:28:LEU:HD11	1:C:42:ARG:HD3	1.95	0.47
1:C:447:ILE:HG21	1:C:520:ILE:HD12	1.96	0.47
1:D:159:HIS:ND1	1:D:190:ARG:HG2	2.30	0.47
1:B:9:PHE:HB3	1:B:120:ASP:CG	2.35	0.47
1:D:425:PHE:CD2	1:D:431:TYR:HA	2.49	0.47
1:B:579:TYR:HB3	1:B:582:LEU:HD21	1.96	0.46
1:A:168:THR:HA	1:A:171:TRP:CD1	2.51	0.46
1:C:98:THR:HG21	1:C:460:GLY:O	2.16	0.46
1:A:421:ARG:NH2	1:A:441:GLU:O	2.48	0.46
1:C:407:ARG:CD	1:C:444:GLU:HG3	2.46	0.46
1:A:168:THR:O	1:A:172:ARG:HG3	2.15	0.46
1:C:325:ARG:HG3	1:C:325:ARG:HH11	1.81	0.46
1:C:407:ARG:HD3	1:C:444:GLU:CG	2.46	0.46
1:C:389:LEU:HA	1:C:510:GLY:HA3	1.97	0.46
1:A:579:TYR:OH	1:B:558:GLU:OE2	2.22	0.46
1:B:57:ILE:O	1:B:91:PHE:HB2	2.16	0.45
1:A:465:VAL:O	1:A:467:MET:N	2.46	0.45
1:D:5:THR:HB	1:D:6:PRO:C	2.37	0.45
1:A:578:LYS:HB3	1:A:578:LYS:HE3	1.77	0.45
1:B:280:ALA:O	1:B:284:ILE:HG13	2.16	0.45
1:C:334:TRP:CE2	1:C:362:GLU:HB2	2.52	0.45
1:A:183:THR:HG23	1:A:185:GLU:H	1.81	0.45
1:A:264:PHE:CZ	1:A:288:ALA:HA	2.52	0.45
1:B:154:MET:HE1	1:B:195:ALA:HB1	1.97	0.45
1:C:472:HIS:HE1	4:C:708:HOH:O	1.99	0.45
1:D:443:ASP:OD2	1:D:445:ARG:N	2.45	0.45
1:A:91:PHE:HZ	1:B:30:ARG:HB3	1.81	0.45
1:A:449:VAL:HA	1:A:484:LEU:O	2.17	0.45
1:A:395:MET:HA	1:A:497:SER:O	2.16	0.45
1:B:424:VAL:HG11	1:B:515:ARG:HA	1.98	0.45
1:D:126:THR:HB	1:D:132:THR:OG1	2.16	0.45
1:B:484:LEU:HD23	1:B:511:LEU:HD21	1.99	0.45
1:D:314:PRO:HD2	4:D:763:HOH:O	2.16	0.45
1:A:91:PHE:CZ	1:B:30:ARG:HB3	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:22:ASP:N	1:C:22:ASP:OD1	2.50	0.44
1:A:317:LYS:HD3	1:A:318:TYR:CE2	2.53	0.44
1:B:19:ASP:N	1:B:19:ASP:OD1	2.48	0.44
1:B:444:GLU:O	1:B:444:GLU:HG2	2.18	0.44
1:B:95:ARG:HG2	1:B:99:ALA:HA	1.98	0.44
1:A:33:ASN:HB2	1:B:154:MET:HE3	2.00	0.44
1:D:22:ASP:OD1	1:D:22:ASP:N	2.50	0.44
1:D:317:LYS:HD3	1:D:318:TYR:CE1	2.53	0.44
1:D:335:GLU:HG3	1:D:372:TYR:HB2	1.99	0.44
1:D:537:THR:O	1:D:541:ARG:HG3	2.17	0.44
1:A:417:VAL:HG12	1:A:523:ASP:HA	1.99	0.44
1:A:4:ARG:HD3	1:A:250:TYR:CE1	2.53	0.43
1:A:143:ASN:OD1	1:A:254:LYS:HB3	2.18	0.43
1:B:156:ASP:OD1	1:B:321:GLU:HB2	2.17	0.43
1:D:136:ILE:HG21	1:D:287:MET:HE3	1.99	0.43
1:B:158:TRP:HA	1:B:162:GLU:O	2.17	0.43
1:B:365:ASP:OD1	1:B:367:GLU:HG3	2.18	0.43
1:B:442:ILE:HD12	1:B:442:ILE:HA	1.71	0.43
1:B:40:GLU:OE2	1:B:76:ARG:NH2	2.49	0.43
1:A:136:ILE:HG21	1:A:287:MET:HE3	2.00	0.43
1:A:417:VAL:HA	1:A:522:ILE:O	2.17	0.43
1:B:279:ASN:O	1:B:282:PRO:HD2	2.19	0.43
1:C:83:MET:HB3	1:C:83:MET:HE2	1.71	0.43
1:C:424:VAL:HG21	1:C:514:LEU:HD23	2.00	0.43
1:D:552:THR:OG1	1:D:561:ARG:HD2	2.19	0.43
1:A:290:HIS:HE1	4:A:736:HOH:O	2.00	0.43
1:B:110:LEU:HD23	1:B:135:GLY:HA2	2.01	0.43
1:B:334:TRP:CZ3	1:B:362:GLU:HG3	2.54	0.43
1:B:486:ASP:HA	1:B:501:ALA:HB3	2.01	0.43
1:A:120:ASP:O	1:A:144:ILE:HB	2.19	0.42
1:A:358:LEU:HD23	1:A:358:LEU:HA	1.83	0.42
1:C:339:GLN:HG3	1:C:372:TYR:CG	2.54	0.42
1:C:95:ARG:HG2	1:C:99:ALA:HA	2.00	0.42
1:D:309:ILE:HD13	1:D:309:ILE:HA	1.71	0.42
1:A:383:LEU:HD23	1:A:524:LEU:HD22	2.01	0.42
1:A:387:GLY:HA3	1:A:529:CYS:O	2.19	0.42
1:C:303:ALA:HA	1:C:306:ILE:HD12	2.00	0.42
1:D:12:ARG:NH2	1:D:42:ARG:HA	2.34	0.42
1:C:390:PHE:CE2	1:C:484:LEU:HD11	2.53	0.42
1:D:227:ILE:HG13	1:D:227:ILE:H	1.71	0.42
1:B:263:ALA:HA	1:B:266:ASN:HD22	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:411:GLN:HA	1:D:412:PRO:HD3	1.92	0.42
1:B:219:LEU:HA	1:B:219:LEU:HD23	1.86	0.42
1:B:384:VAL:HG12	1:B:394:ILE:HG22	2.01	0.42
1:B:473:LEU:HD23	1:B:473:LEU:HA	1.76	0.42
1:A:143:ASN:ND2	1:A:254:LYS:HD3	2.33	0.42
1:A:281:GLN:HB3	1:A:282:PRO:HD3	2.02	0.42
1:B:409:LEU:HD21	1:B:415:GLU:CA	2.46	0.42
1:B:502:SER:HA	1:B:503:PRO:C	2.39	0.42
1:C:170:ILE:O	1:C:174:ARG:HG3	2.20	0.42
1:C:461:SER:OG	1:C:488:ARG:NE	2.36	0.42
1:A:325:ARG:HD2	1:D:158:TRP:HB2	2.02	0.42
1:A:12:ARG:CZ	1:A:44:GLY:HA2	2.50	0.42
1:A:197:SER:O	1:B:33:ASN:HB2	2.19	0.42
1:C:182:ILE:HB	1:C:186:GLU:HG3	2.01	0.42
1:C:389:LEU:HD11	1:C:514:LEU:HD13	2.01	0.42
1:A:105:LEU:HB2	1:A:556:TRP:CE2	2.55	0.42
1:A:32:MET:HE3	1:C:236:GLN:HE22	1.85	0.42
1:C:425:PHE:CD1	1:C:431:TYR:HA	2.55	0.42
1:A:331:ALA:HA	1:A:361:ARG:O	2.20	0.41
1:A:509:GLY:O	1:A:512:SER:OG	2.27	0.41
1:B:445:ARG:HE	1:B:445:ARG:HB2	1.59	0.41
1:C:200:HIS:HB2	3:C:602:FES:S2	2.60	0.41
1:B:406:LYS:HA	1:B:410:SER:OG	2.20	0.41
1:C:444:GLU:HG2	1:C:445:ARG:HD2	2.01	0.41
1:A:147:ILE:HD13	1:A:241:THR:HG23	2.01	0.41
1:A:12:ARG:HH12	1:A:42:ARG:HA	1.84	0.41
1:B:289:ARG:NH1	1:B:569:THR:HB	2.36	0.41
1:B:281:GLN:HA	1:B:300:TRP:CZ2	2.55	0.41
1:C:537:THR:HG22	1:C:541:ARG:HD2	2.01	0.41
1:C:537:THR:O	1:C:541:ARG:HD2	2.20	0.41
1:A:390:PHE:CE2	1:A:484:LEU:HD11	2.52	0.41
1:B:523:ASP:OD1	1:B:526:THR:N	2.34	0.41
1:C:387:GLY:HA3	1:C:529:CYS:O	2.21	0.41
1:A:586:LEU:HA	1:A:586:LEU:HD23	1.89	0.41
1:C:352:LYS:HB3	1:C:356:GLU:HB2	2.01	0.41
1:D:339:GLN:HG3	1:D:372:TYR:CD1	2.56	0.41
1:A:174:ARG:HD3	1:B:22:ASP:OD2	2.20	0.41
1:B:409:LEU:HD22	1:B:409:LEU:HA	1.78	0.41
1:A:70:ARG:NH2	1:C:36:ILE:HA	2.35	0.41
1:D:309:ILE:HD11	1:D:372:TYR:HA	2.02	0.41
1:C:84:GLU:O	1:D:56:ASP:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:317:LYS:NZ	1:A:318:TYR:OH	2.42	0.41
1:B:39:GLU:O	1:B:43:SER:HB3	2.20	0.41
1:C:32:MET:HB3	1:C:32:MET:HE2	1.80	0.41
1:C:53:THR:CB	1:C:61:ASN:HD22	2.34	0.41
1:B:114:LEU:HD22	1:B:144:ILE:HD11	2.02	0.41
1:B:466:ASN:HB3	1:B:489:GLN:OE1	2.21	0.41
1:B:306:ILE:HD11	1:B:341:ARG:NH1	2.36	0.41
1:B:17:ASN:HD22	1:B:20:HIS:H	1.69	0.40
1:B:309:ILE:HA	1:B:309:ILE:HD13	1.78	0.40
1:B:577:VAL:H	1:B:577:VAL:HG23	1.65	0.40
1:B:53:THR:HB	1:B:61:ASN:HD22	1.86	0.40
1:C:407:ARG:HD3	1:C:444:GLU:CD	2.41	0.40
1:A:153:PRO:HD2	1:A:228:PRO:HA	2.04	0.40
1:A:26:LEU:HD23	1:B:170:ILE:HG13	2.03	0.40
1:A:354:MET:HE2	1:A:358:LEU:HD11	2.03	0.40
1:A:105:LEU:HD21	1:B:109:GLY:HA2	2.04	0.40
1:B:384:VAL:HA	1:B:393:ALA:O	2.20	0.40
1:C:339:GLN:HG3	1:C:372:TYR:CD1	2.56	0.40
1:A:227:ILE:H	1:A:227:ILE:HG13	1.77	0.40
1:A:401:GLY:HA3	4:A:756:HOH:O	2.21	0.40
1:B:389:LEU:HA	1:B:510:GLY:HA3	2.03	0.40
1:D:395:MET:HA	1:D:497:SER:O	2.21	0.40
1:C:14:TRP:CZ2	1:D:96:ARG:HD3	2.56	0.40
1:D:484:LEU:HD12	1:D:498:ILE:HB	2.04	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	586/600 (98%)	567 (97%)	17 (3%)	2 (0%)	41 66

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	586/600 (98%)	549 (94%)	30 (5%)	7 (1%)	13	32
1	C	585/600 (98%)	557 (95%)	25 (4%)	3 (0%)	29	54
1	D	585/600 (98%)	563 (96%)	20 (3%)	2 (0%)	41	66
All	All	2342/2400 (98%)	2236 (96%)	92 (4%)	14 (1%)	25	50

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	161	ASN
1	C	225	ALA
1	A	460	GLY
1	B	129	ASP
1	B	460	GLY
1	C	129	ASP
1	D	129	ASP
1	B	581	ASP
1	C	460	GLY
1	A	127	GLY
1	B	363	THR
1	B	477	GLY
1	B	127	GLY
1	D	127	GLY

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	468/479 (98%)	463 (99%)	5 (1%)	73	90
1	B	468/479 (98%)	455 (97%)	13 (3%)	43	73
1	C	467/479 (98%)	453 (97%)	14 (3%)	41	70
1	D	467/479 (98%)	457 (98%)	10 (2%)	53	80
All	All	1870/1916 (98%)	1828 (98%)	42 (2%)	52	79

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	193	SER
1	A	232	ARG
1	A	402	GLU
1	A	411	GLN
1	A	529	CYS
1	B	8	ARG
1	B	10	ARG
1	B	77	ASP
1	B	193	SER
1	B	232	ARG
1	B	270	LEU
1	B	294	GLU
1	B	341	ARG
1	B	359	GLN
1	B	428	SER
1	B	445	ARG
1	B	528	ARG
1	B	529	CYS
1	C	7	ARG
1	C	8	ARG
1	C	12	ARG
1	C	29	GLU
1	C	31	PHE
1	C	66	ASP
1	C	187	PHE
1	C	190	ARG
1	C	193	SER
1	C	359	GLN
1	C	376	LEU
1	C	410	SER
1	C	433	LYS
1	C	451	ARG
1	D	4	ARG
1	D	26	LEU
1	D	31	PHE
1	D	33	ASN
1	D	58	SER
1	D	187	PHE
1	D	193	SER
1	D	270	LEU
1	D	312	MET
1	D	470	PRO

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	17	ASN
1	C	262	GLN
1	C	343	HIS
1	C	414	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

4 non-standard protein/DNA/RNA residues 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	$\#\|Z\| > 2$
1	KCX	C	130	1,2	7,11,12	1.20	1 (14%)	4,12,14	0.75	0
1	KCX	A	130	1,2	7,11,12	0.89	0	4,12,14	0.66	0
1	KCX	D	130	1,2	7,11,12	1.19	1 (14%)	4,12,14	1.32	1 (25%)
1	KCX	B	130	1,2	7,11,12	1.03	1 (14%)	4,12,14	0.73	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
1	KCX	C	130	1,2	-	1/7/10/12	-
1	KCX	A	130	1,2	-	3/7/10/12	-
1	KCX	D	130	1,2	-	3/7/10/12	-
1	KCX	B	130	1,2	-	1/7/10/12	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	130	KCX	CE-NZ	2.89	1.51	1.45
1	C	130	KCX	CE-NZ	2.69	1.51	1.45
1	B	130	KCX	CE-NZ	2.45	1.51	1.45

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	130	KCX	CD-CE-NZ	-2.55	104.64	111.49

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	C	130	KCX	C-CA-CB-CG
1	A	130	KCX	C-CA-CB-CG
1	D	130	KCX	C-CA-CB-CG
1	B	130	KCX	C-CA-CB-CG
1	A	130	KCX	CG-CD-CE-NZ
1	D	130	KCX	CA-CB-CG-CD
1	D	130	KCX	CG-CD-CE-NZ
1	A	130	KCX	CA-CB-CG-CD

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	D	130	KCX	1	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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	FES	D	602	1,4	0,4,4	0.00	-	-		
3	FES	B	602	1	0,4,4	0.00	-	-		
3	FES	C	602	1	0,4,4	0.00	-	-		
3	FES	A	602	1	0,4,4	0.00	-	-		

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	FES	D	602	1,4	-	-	0/1/1/1
3	FES	B	602	1	-	-	0/1/1/1
3	FES	C	602	1	-	-	0/1/1/1
3	FES	A	602	1	-	-	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	602	FES	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, 95^{th} 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	588/600 (98%)	0.01	34 (5%)	23 22	42, 64, 88, 111	0
1	B	588/600 (98%)	0.25	52 (8%)	10 8	48, 76, 118, 134	0
1	C	587/600 (97%)	-0.11	13 (2%)	62 63	45, 61, 85, 106	0
1	D	587/600 (97%)	-0.16	12 (2%)	65 67	39, 56, 84, 104	0
All	All	2350/2400 (97%)	-0.00	111 (4%)	31 30	39, 63, 103, 134	0

All (111) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	179	ALA	7.2
1	B	539	ALA	5.4
1	B	412	PRO	4.9
1	B	536	ALA	4.8
1	B	410	SER	4.8
1	C	536	ALA	4.8
1	B	472	HIS	4.8
1	A	439	ALA	4.5
1	B	183	THR	4.1
1	B	182	ILE	4.0
1	B	406	LYS	4.0
1	A	414	GLN	3.9
1	B	521	ARG	3.9
1	B	411	GLN	3.9
1	D	4	ARG	3.7
1	B	533	VAL	3.7
1	B	540	ALA	3.6
1	B	3	ASN	3.6
1	B	475	LYS	3.6
1	B	181	GLU	3.6
1	C	184	GLU	3.6

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Mol	Chain	Res	Type	RSRZ
1	D	181	GLU	3.5
1	A	536	ALA	3.5
1	B	180	GLY	3.5
1	A	182	ILE	3.5
1	A	545	GLY	3.4
1	B	188	ILE	3.4
1	A	543	GLN	3.3
1	B	534	ASP	3.3
1	B	415	GLU	3.3
1	B	184	GLU	3.3
1	B	545	GLY	3.2
1	A	183	THR	3.1
1	A	3	ASN	3.1
1	B	541	ARG	3.1
1	B	185	GLU	3.1
1	D	185	GLU	3.1
1	B	438	PRO	3.1
1	D	182	ILE	3.1
1	B	378	GLU	3.1
1	B	186	GLU	3.0
1	B	413	GLY	3.0
1	D	183	THR	3.0
1	C	18	PRO	3.0
1	A	438	PRO	2.9
1	A	538	ILE	2.9
1	A	466	ASN	2.9
1	B	414	GLN	2.9
1	B	187	PHE	2.9
1	D	543	GLN	2.9
1	C	6	PRO	2.9
1	A	412	PRO	2.8
1	D	545	GLY	2.8
1	D	5	THR	2.8
1	A	184	GLU	2.7
1	B	437	ASP	2.7
1	B	465	VAL	2.7
1	B	433	LYS	2.7
1	A	19	ASP	2.7
1	A	179	ALA	2.7
1	B	538	ILE	2.6
1	A	374	GLU	2.6
1	A	185	GLU	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	294	GLU	2.6
1	C	182	ILE	2.6
1	D	180	GLY	2.6
1	B	483	THR	2.6
1	D	7	ARG	2.6
1	A	465	VAL	2.5
1	A	437	ASP	2.5
1	A	539	ALA	2.5
1	C	185	GLU	2.5
1	C	534	ASP	2.5
1	A	178	ALA	2.4
1	A	534	ASP	2.4
1	A	483	THR	2.4
1	C	5	THR	2.4
1	A	533	VAL	2.4
1	B	294	GLU	2.4
1	B	532	LEU	2.4
1	C	537	THR	2.4
1	B	485	GLY	2.3
1	A	495	SER	2.3
1	A	541	ARG	2.3
1	C	538	ILE	2.3
1	B	548	ALA	2.3
1	B	178	ALA	2.2
1	B	537	THR	2.2
1	A	18	PRO	2.2
1	B	439	ALA	2.2
1	B	498	ILE	2.2
1	D	540	ALA	2.2
1	B	441	GLU	2.2
1	C	374	GLU	2.2
1	B	370	PHE	2.2
1	B	417	VAL	2.1
1	A	489	GLN	2.1
1	B	403	GLU	2.1
1	B	479	MET	2.1
1	C	183	THR	2.1
1	A	537	THR	2.1
1	A	180	GLY	2.1
1	A	181	GLU	2.1
1	B	21	ILE	2.1
1	C	466	ASN	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	450	ILE	2.0
1	D	184	GLU	2.0
1	A	476	LYS	2.0
1	A	544	ASP	2.0
1	B	543	GLN	2.0
1	B	474	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (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, 95^{th} 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
1	KCX	B	130	12/13	0.88	0.22	62,71,85,86	0
1	KCX	A	130	12/13	0.91	0.23	59,66,80,81	0
1	KCX	C	130	12/13	0.92	0.18	51,56,68,69	0
1	KCX	D	130	12/13	0.93	0.23	44,54,77,78	0

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. The B-factors column lists the minimum, median, 95^{th} 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	MG	C	601	1/1	0.78	0.11	71,71,71,71	0
2	MG	D	601	1/1	0.82	0.21	93,93,93,93	0
2	MG	B	601	1/1	0.86	0.08	86,86,86,86	0
2	MG	A	601	1/1	0.91	0.14	79,79,79,79	0
3	FES	A	602	4/4	0.99	0.07	56,67,73,79	0
3	FES	D	602	4/4	0.99	0.07	60,64,65,77	0
3	FES	C	602	4/4	0.99	0.09	64,69,76,77	0
3	FES	B	602	4/4	0.99	0.07	85,85,90,104	0

6.5 Other polymers (i)

There are no such residues in this entry.