Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:10 AM GMT

PDB ID	:	2FVK
Title	:	Crystal structure of dihydropyrimidinase from Saccharomyces kluyveri in complex with the substrate dihydrouracil
Authors	:	Dobritzsch, D.; Lohkamp, B.
Deposited on	:	2006-01-31
Resolution	:	2.40 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 ①) were used in the production of this report:

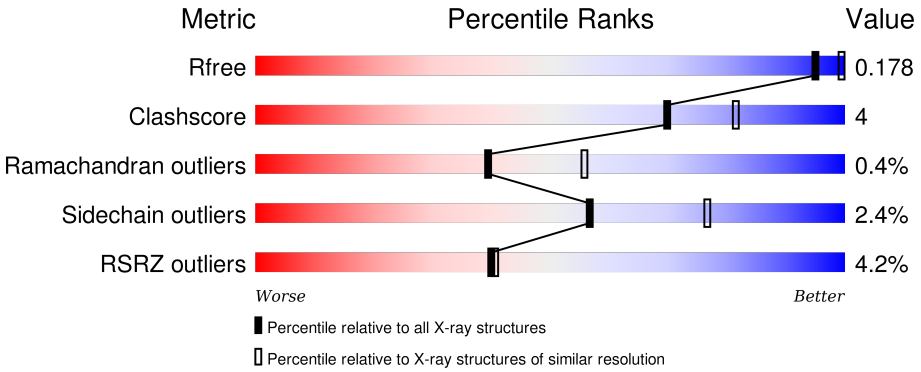
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 2.40 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}	91344	2919 (2.40-2.40)
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (2.40-2.40)

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 <=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	559	4% 83% 12% 5%
1	B	559	3% 83% 11% • 5%
1	C	559	4% 81% 13% • 5%
1	D	559	5% 84% 10% • 5%

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	ZN	A	602	-	-	-	X
2	ZN	B	602	-	-	-	X
2	ZN	C	602	-	-	-	X
2	ZN	D	602	-	-	-	X
3	DUC	A	604	-	-	-	X
3	DUC	B	604	-	-	-	X
3	DUC	D	604	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 17698 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	532	Total	C	N	O	S	0	1	0
			4155	2638	680	810	27			
1	B	532	Total	C	N	O	S	0	1	0
			4152	2637	680	808	27			
1	C	531	Total	C	N	O	S	0	1	0
			4142	2631	677	807	27			
1	D	532	Total	C	N	O	S	0	2	0
			4166	2647	680	812	27			

There are 76 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	167	KCX	LYS	MODIFIED RESIDUE	UNP Q9P903
A	543	PRO	-	EXPRESSION TAG	UNP Q9P903
A	544	GLY	-	EXPRESSION TAG	UNP Q9P903
A	545	ASP	-	EXPRESSION TAG	UNP Q9P903
A	546	ASP	-	EXPRESSION TAG	UNP Q9P903
A	547	ASP	-	EXPRESSION TAG	UNP Q9P903
A	548	ASP	-	EXPRESSION TAG	UNP Q9P903
A	549	LYS	-	EXPRESSION TAG	UNP Q9P903
A	550	HIS	-	EXPRESSION TAG	UNP Q9P903
A	551	HIS	-	EXPRESSION TAG	UNP Q9P903
A	552	HIS	-	EXPRESSION TAG	UNP Q9P903
A	553	HIS	-	EXPRESSION TAG	UNP Q9P903
A	554	HIS	-	EXPRESSION TAG	UNP Q9P903
A	555	HIS	-	EXPRESSION TAG	UNP Q9P903
A	556	HIS	-	EXPRESSION TAG	UNP Q9P903
A	557	HIS	-	EXPRESSION TAG	UNP Q9P903
A	558	SER	-	EXPRESSION TAG	UNP Q9P903
A	559	GLY	-	EXPRESSION TAG	UNP Q9P903
A	560	ASP	-	EXPRESSION TAG	UNP Q9P903
B	167	KCX	LYS	MODIFIED RESIDUE	UNP Q9P903
B	543	PRO	-	EXPRESSION TAG	UNP Q9P903

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Chain	Residue	Modelled	Actual	Comment	Reference
B	544	GLY	-	EXPRESSION TAG	UNP Q9P903
B	545	ASP	-	EXPRESSION TAG	UNP Q9P903
B	546	ASP	-	EXPRESSION TAG	UNP Q9P903
B	547	ASP	-	EXPRESSION TAG	UNP Q9P903
B	548	ASP	-	EXPRESSION TAG	UNP Q9P903
B	549	LYS	-	EXPRESSION TAG	UNP Q9P903
B	550	HIS	-	EXPRESSION TAG	UNP Q9P903
B	551	HIS	-	EXPRESSION TAG	UNP Q9P903
B	552	HIS	-	EXPRESSION TAG	UNP Q9P903
B	553	HIS	-	EXPRESSION TAG	UNP Q9P903
B	554	HIS	-	EXPRESSION TAG	UNP Q9P903
B	555	HIS	-	EXPRESSION TAG	UNP Q9P903
B	556	HIS	-	EXPRESSION TAG	UNP Q9P903
B	557	HIS	-	EXPRESSION TAG	UNP Q9P903
B	558	SER	-	EXPRESSION TAG	UNP Q9P903
B	559	GLY	-	EXPRESSION TAG	UNP Q9P903
B	560	ASP	-	EXPRESSION TAG	UNP Q9P903
C	167	KCX	LYS	MODIFIED RESIDUE	UNP Q9P903
C	543	PRO	-	EXPRESSION TAG	UNP Q9P903
C	544	GLY	-	EXPRESSION TAG	UNP Q9P903
C	545	ASP	-	EXPRESSION TAG	UNP Q9P903
C	546	ASP	-	EXPRESSION TAG	UNP Q9P903
C	547	ASP	-	EXPRESSION TAG	UNP Q9P903
C	548	ASP	-	EXPRESSION TAG	UNP Q9P903
C	549	LYS	-	EXPRESSION TAG	UNP Q9P903
C	550	HIS	-	EXPRESSION TAG	UNP Q9P903
C	551	HIS	-	EXPRESSION TAG	UNP Q9P903
C	552	HIS	-	EXPRESSION TAG	UNP Q9P903
C	553	HIS	-	EXPRESSION TAG	UNP Q9P903
C	554	HIS	-	EXPRESSION TAG	UNP Q9P903
C	555	HIS	-	EXPRESSION TAG	UNP Q9P903
C	556	HIS	-	EXPRESSION TAG	UNP Q9P903
C	557	HIS	-	EXPRESSION TAG	UNP Q9P903
C	558	SER	-	EXPRESSION TAG	UNP Q9P903
C	559	GLY	-	EXPRESSION TAG	UNP Q9P903
C	560	ASP	-	EXPRESSION TAG	UNP Q9P903
D	167	KCX	LYS	MODIFIED RESIDUE	UNP Q9P903
D	543	PRO	-	EXPRESSION TAG	UNP Q9P903
D	544	GLY	-	EXPRESSION TAG	UNP Q9P903
D	545	ASP	-	EXPRESSION TAG	UNP Q9P903
D	546	ASP	-	EXPRESSION TAG	UNP Q9P903
D	547	ASP	-	EXPRESSION TAG	UNP Q9P903

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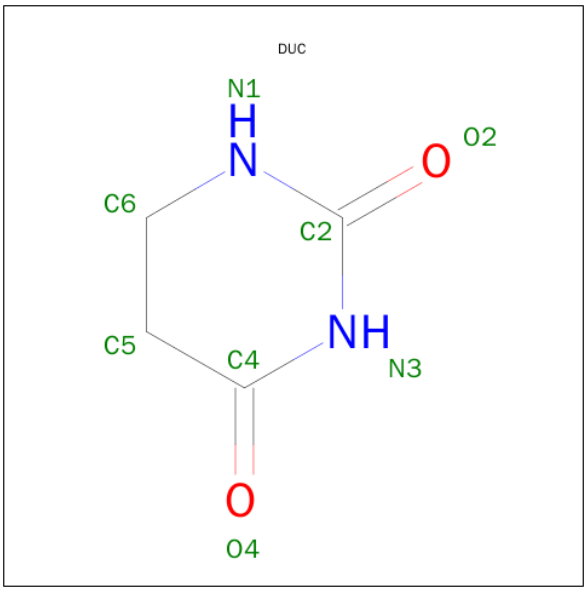
Chain	Residue	Modelled	Actual	Comment	Reference
D	548	ASP	-	EXPRESSION TAG	UNP Q9P903
D	549	LYS	-	EXPRESSION TAG	UNP Q9P903
D	550	HIS	-	EXPRESSION TAG	UNP Q9P903
D	551	HIS	-	EXPRESSION TAG	UNP Q9P903
D	552	HIS	-	EXPRESSION TAG	UNP Q9P903
D	553	HIS	-	EXPRESSION TAG	UNP Q9P903
D	554	HIS	-	EXPRESSION TAG	UNP Q9P903
D	555	HIS	-	EXPRESSION TAG	UNP Q9P903
D	556	HIS	-	EXPRESSION TAG	UNP Q9P903
D	557	HIS	-	EXPRESSION TAG	UNP Q9P903
D	558	SER	-	EXPRESSION TAG	UNP Q9P903
D	559	GLY	-	EXPRESSION TAG	UNP Q9P903
D	560	ASP	-	EXPRESSION TAG	UNP Q9P903

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

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

- Molecule 3 is DIHYDROPYRIMIDINE-2,4(1H,3H)-DIONE (three-letter code: DUC) (formula: $C_4H_6N_2O_2$).



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

- Molecule 4 is water.

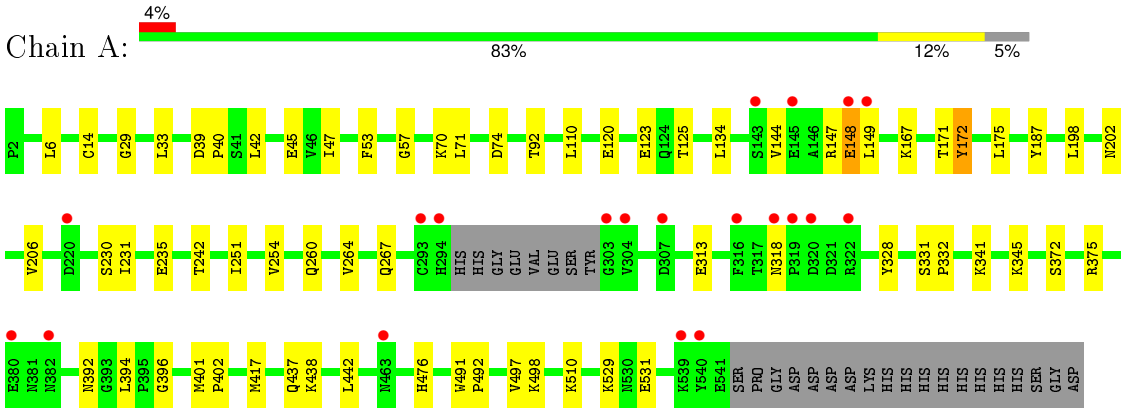
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	282	Total O 282 282	0	0
4	B	251	Total O 251 251	0	0
4	C	265	Total O 265 265	0	0
4	D	245	Total O 245 245	0	0

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 errors 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.

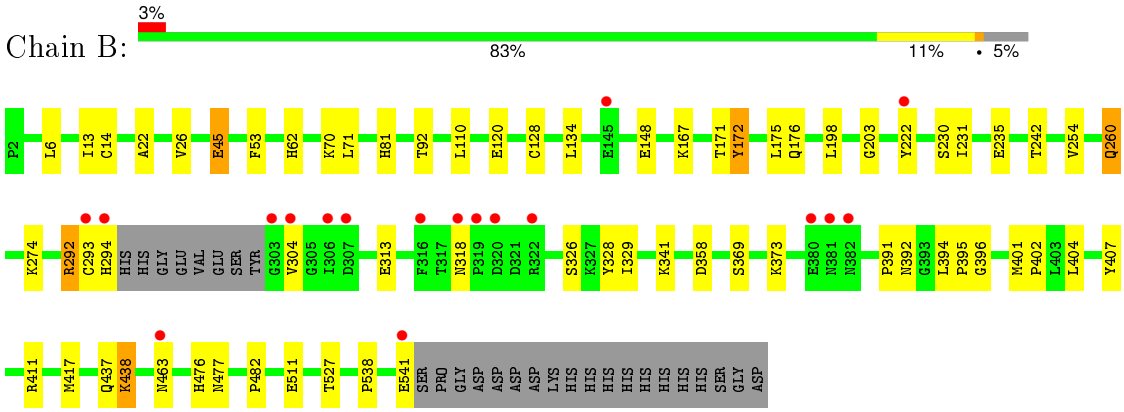
- Molecule 1: dihydropyrimidinase

Chain A:



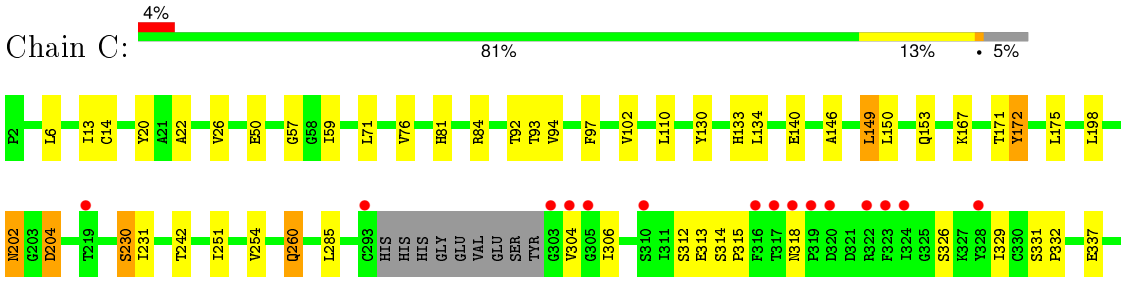
- Molecule 1: dihydropyrimidinase

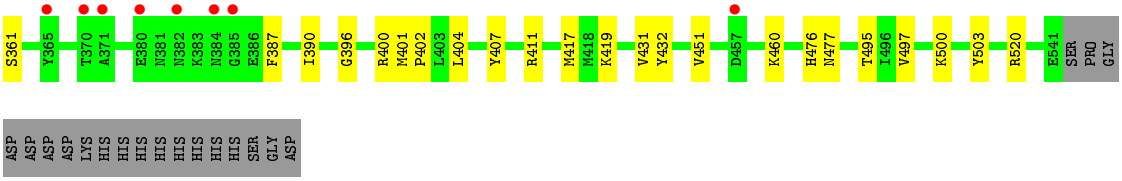
Chain B:



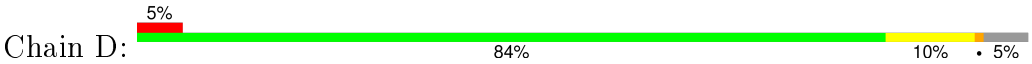
- Molecule 1: dihydropyrimidinase

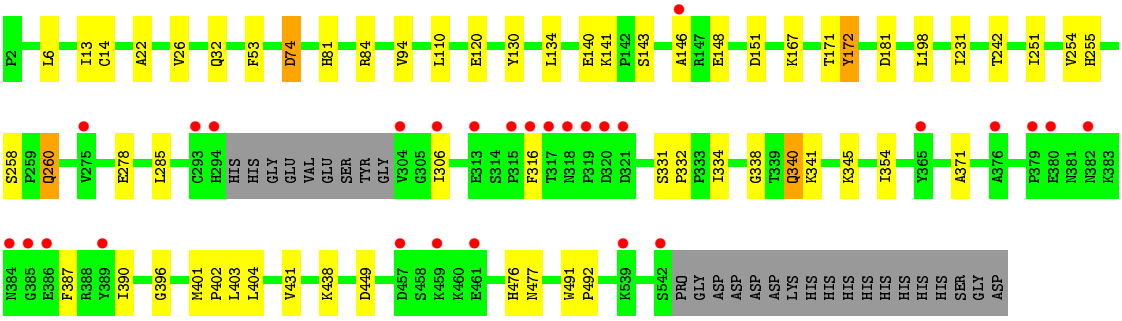
Chain C:





- Molecule 1: dihydropyrimidinase





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	90.13Å 71.60Å 161.89Å 90.00° 91.40° 90.00°	Depositor
Resolution (Å)	54.23 – 2.40 53.62 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.1 (54.23-2.40) 99.1 (53.62-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [1]	1.91 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.178 , 0.234 0.184 , 0.178	Depositor DCC
R_{free} test set	4042 reflections (5.30%)	DCC
Wilson B-factor (Å^2)	31.7	Xtriage
Anisotropy	0.530	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 44.3	EDS
Estimated twinning fraction	0.139 for h,-k,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.30$	Xtriage
Outliers	1 of 80364 reflections (0.001%)	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	17698	wwPDB-VP
Average B, all atoms (Å^2)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.01% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: ZN, DUC, 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	0.47	0/4239	0.58	1/5752 (0.0%)
1	B	0.44	0/4239	0.58	1/5752 (0.0%)
1	C	0.44	0/4228	0.58	0/5737
1	D	0.43	0/4254	0.58	0/5774
All	All	0.45	0/16960	0.58	2/23015 (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	B	394	LEU	CA-CB-CG	5.63	128.25	115.30
1	A	33	LEU	CA-CB-CG	5.01	126.82	115.30

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	4155	0	4084	39	0
1	B	4152	0	4083	34	0
1	C	4142	0	4076	44	0
1	D	4166	0	4095	37	0
2	A	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
3	A	8	0	6	0	0
3	B	8	0	6	0	0
3	C	8	0	6	0	0
3	D	8	0	6	0	0
4	A	282	0	0	1	0
4	B	251	0	0	0	0
4	C	265	0	0	4	0
4	D	245	0	0	1	0
All	All	17698	0	16362	147	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 4.

All (147) 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:198:LEU:HD12	1:A:251:ILE:HD11	1.49	0.93
1:C:140:GLU:O	1:C:146:ALA:HB2	1.78	0.84
1:B:230:SER:HB3	1:B:260:GLN:HE22	1.44	0.83
1:D:140:GLU:O	1:D:146:ALA:CB	2.27	0.83
1:D:140:GLU:O	1:D:146:ALA:HB2	1.80	0.81
1:B:274:LYS:HE3	1:B:527:THR:O	1.81	0.81
1:D:198:LEU:HD12	1:D:251:ILE:HD11	1.62	0.80
1:C:260:GLN:HE21	1:C:260:GLN:H	1.32	0.76
1:A:231:ILE:HG12	1:B:242:THR:HG23	1.66	0.76
1:D:285:LEU:HB3	1:D:306:ILE:HD12	1.72	0.71
1:A:242:THR:HG23	1:B:231:ILE:HG12	1.71	0.71
1:A:123:GLU:OE1	1:A:123:GLU:HA	1.91	0.69
1:C:14[B]:CYS:SG	1:C:417:MET:HB3	2.33	0.68
1:B:171:THR:O	1:B:172:TYR:HB2	1.95	0.65
1:A:144:VAL:HA	1:A:147:ARG:HG3	1.78	0.64
1:D:140:GLU:O	1:D:146:ALA:HB1	1.97	0.64
1:B:230:SER:HB3	1:B:260:GLN:NE2	2.11	0.63
1:C:285:LEU:HB3	1:C:306:ILE:HD12	1.80	0.62
1:C:326:SER:HA	1:C:329:ILE:HG12	1.82	0.62
1:C:71:LEU:HD11	1:C:175:LEU:HD21	1.83	0.61
1:C:198:LEU:HD23	1:C:251:ILE:HD11	1.82	0.60
1:A:14[A]:CYS:SG	1:A:53:PHE:CD2	2.95	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:387:PHE:HA	1:C:390:ILE:HD12	1.84	0.60
1:C:140:GLU:O	1:C:146:ALA:CB	2.49	0.58
1:A:71:LEU:HD11	1:A:175:LEU:HD21	1.86	0.58
1:D:340:GLN:CD	1:D:340:GLN:H	2.06	0.57
1:C:13:ILE:HD12	1:C:22:ALA:HB3	1.87	0.57
1:D:110:LEU:HB3	1:D:134:LEU:HD21	1.87	0.56
1:B:538:PRO:HD2	1:B:541:GLU:HG3	1.88	0.55
1:A:198:LEU:HD12	1:A:251:ILE:CD1	2.30	0.55
1:B:222:TYR:CD1	1:B:292:ARG:HG2	2.42	0.54
1:B:373:LYS:HD3	1:B:391:PRO:HG2	1.90	0.54
1:A:264:VAL:HA	1:A:267:GLN:HE21	1.73	0.54
1:A:167:KCX:HE2	1:A:254:VAL:HG21	1.90	0.53
1:D:172[A]:TYR:OH	1:D:331:SER:HB2	2.08	0.53
1:D:198:LEU:HD12	1:D:251:ILE:CD1	2.36	0.53
1:C:149:LEU:HD22	1:C:153:GLN:HG3	1.91	0.53
1:C:313:GLU:HA	1:C:318:ASN:HD21	1.74	0.53
1:B:326:SER:HA	1:B:329:ILE:HG12	1.91	0.53
1:C:230:SER:HB3	1:C:260:GLN:HE22	1.74	0.52
1:C:313:GLU:HA	1:C:318:ASN:ND2	2.25	0.52
1:C:407:TYR:HA	1:C:411:ARG:HD2	1.92	0.51
1:A:171:THR:O	1:A:172:TYR:HB2	2.10	0.51
1:B:304:VAL:HG11	1:B:341:LYS:HG3	1.93	0.51
1:A:442:LEU:HD22	1:C:20:TYR:CE2	2.46	0.51
1:C:230:SER:HB3	1:C:260:GLN:NE2	2.27	0.50
1:D:341:LYS:HE3	1:D:345:LYS:HE3	1.94	0.50
1:C:92:THR:HG22	1:C:497:VAL:HG22	1.93	0.50
1:D:285:LEU:HD13	1:D:403:LEU:HD22	1.93	0.50
1:A:172:TYR:OH	1:A:331:SER:HB2	2.11	0.50
1:B:71:LEU:HD11	1:B:175:LEU:HD21	1.93	0.50
1:D:278:GLU:HG3	1:D:354:ILE:HG13	1.91	0.50
1:C:202:ASN:C	1:C:202:ASN:HD22	2.15	0.50
1:C:242:THR:HG23	1:D:231:ILE:HG12	1.93	0.50
1:D:141:LYS:NZ	1:D:181:ASP:OD2	2.45	0.49
1:D:491:TRP:CD1	1:D:492:PRO:HD2	2.46	0.49
1:C:314:SER:HB2	1:C:315:PRO:HD2	1.95	0.49
1:B:110:LEU:HB3	1:B:134:LEU:HD21	1.94	0.49
1:A:230:SER:HB3	1:A:260:GLN:HE22	1.77	0.49
1:B:437:GLN:HG2	1:B:438:LYS:HD2	1.95	0.49
1:B:13:ILE:HD12	1:B:22:ALA:HB3	1.95	0.49
1:D:438:LYS:NZ	1:D:449:ASP:OD2	2.42	0.48
1:A:74:ASP:O	1:A:375:ARG:NH2	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:102:VAL:HG22	4:C:624:HOH:O	2.13	0.48
1:D:401:MET:HB2	1:D:402:PRO:HD3	1.95	0.48
1:A:39:ASP:HB3	1:A:42:LEU:HG	1.96	0.48
1:A:401:MET:HB2	1:A:402:PRO:HD3	1.95	0.48
1:C:167:KCX:HE2	1:C:254:VAL:HG21	1.96	0.48
1:B:14[A]:CYS:SG	1:B:53:PHE:CD2	3.07	0.47
1:D:143:SER:HA	1:D:146:ALA:HB3	1.97	0.47
1:A:230:SER:CB	1:A:260:GLN:HE22	2.27	0.47
1:D:167:KCX:HE2	1:D:254:VAL:HG21	1.96	0.47
1:C:231:ILE:HG12	1:D:242:THR:HG23	1.96	0.47
1:B:167:KCX:HE2	1:B:254:VAL:HG21	1.97	0.47
1:C:400:ARG:HD3	4:C:606:HOH:O	2.14	0.47
1:C:146:ALA:O	1:C:150:LEU:HB2	2.15	0.46
1:B:313:GLU:HA	1:B:318:ASN:ND2	2.29	0.46
1:D:6:LEU:HB3	1:D:26:VAL:HB	1.97	0.46
1:A:125:THR:HG21	1:A:510:LYS:HZ2	1.81	0.46
1:B:62:HIS:CD2	1:B:358:ASP:HA	2.51	0.46
1:A:149:LEU:HB3	4:A:708:HOH:O	2.15	0.46
1:A:437:GLN:HG2	1:A:438:LYS:HD2	1.97	0.45
1:C:84:ARG:HD3	4:C:664:HOH:O	2.15	0.45
1:C:81:HIS:CG	1:C:477:ASN:HB2	2.52	0.45
1:C:6:LEU:HB3	1:C:26:VAL:HB	1.99	0.45
1:B:407:TYR:HA	1:B:411:ARG:HD2	1.98	0.45
1:B:6:LEU:HB3	1:B:26:VAL:HB	1.99	0.45
1:D:338:GLY:N	1:D:340:GLN:OE1	2.47	0.45
1:B:260:GLN:H	1:B:260:GLN:NE2	2.15	0.44
1:A:372:SER:O	1:A:375:ARG:HB2	2.17	0.44
1:C:57:GLY:HA2	1:C:451:VAL:HG23	1.99	0.44
1:D:316:PHE:CD2	1:D:316:PHE:N	2.86	0.44
1:C:59:ILE:HG12	1:C:93:THR:HB	2.00	0.44
1:C:202:ASN:HD21	1:C:204:ASP:HB2	1.83	0.44
1:D:387:PHE:HA	1:D:390:ILE:HD12	2.00	0.44
1:B:81:HIS:CG	1:B:477:ASN:HB2	2.52	0.44
1:A:148:GLU:HA	1:A:148:GLU:OE2	2.18	0.43
1:C:94:VAL:O	1:C:130:TYR:HA	2.18	0.43
1:C:331:SER:HA	1:C:332:PRO:C	2.38	0.43
1:D:285:LEU:HB3	1:D:306:ILE:CD1	2.44	0.43
1:A:110:LEU:HB3	1:A:134:LEU:HD21	2.00	0.43
1:A:328:TYR:HA	1:A:394:LEU:CD2	2.48	0.43
1:C:110:LEU:HB3	1:C:134:LEU:HD21	2.00	0.43
1:D:171:THR:O	1:D:172[A]:TYR:HB2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:235:GLU:HB2	1:B:242:THR:HG21	2.01	0.43
1:D:316:PHE:N	1:D:316:PHE:HD2	2.17	0.43
1:A:491:TRP:CD1	1:A:492:PRO:HD2	2.54	0.43
1:C:401:MET:HB2	1:C:402:PRO:HD3	2.00	0.43
1:A:147:ARG:HD2	1:A:187:TYR:CE2	2.54	0.42
1:D:74:ASP:HB3	1:D:371:ALA:HB2	2.00	0.42
1:D:258:SER:OG	1:D:260:GLN:HG2	2.19	0.42
1:B:293:CYS:O	1:B:294:HIS:HB2	2.18	0.42
1:A:313:GLU:HA	1:A:318:ASN:ND2	2.33	0.42
1:C:97:PHE:CD2	1:C:133:HIS:HB2	2.54	0.42
1:D:84:ARG:HD3	4:D:739:HOH:O	2.18	0.42
1:D:94:VAL:O	1:D:130:TYR:HA	2.20	0.42
1:B:14[B]:CYS:SG	1:B:417:MET:HB3	2.59	0.42
1:D:148:GLU:O	1:D:151:ASP:HB3	2.19	0.42
1:A:331:SER:HA	1:A:332:PRO:C	2.40	0.42
1:A:57:GLY:HA3	1:A:92:THR:OG1	2.20	0.42
1:C:50:GLU:OE1	1:C:460:LYS:NZ	2.53	0.42
1:B:62:HIS:HD2	1:B:358:ASP:HA	1.82	0.42
1:B:293:CYS:O	1:B:294:HIS:CB	2.68	0.42
1:C:495:THR:HB	1:C:503:TYR:HB3	2.02	0.42
1:C:171:THR:O	1:C:172:TYR:HB2	2.19	0.42
1:A:242:THR:HG21	1:B:235:GLU:HB2	2.01	0.41
1:B:92:THR:O	1:B:128:CYS:HB2	2.20	0.41
1:D:491:TRP:CG	1:D:492:PRO:HD2	2.56	0.41
1:D:331:SER:HA	1:D:332:PRO:C	2.40	0.41
1:C:387:PHE:HA	1:C:390:ILE:CD1	2.49	0.41
1:A:202:ASN:O	1:A:206:VAL:HG23	2.20	0.41
1:D:81:HIS:CG	1:D:477:ASN:HB2	2.56	0.41
1:C:76:VAL:HG22	1:C:361:SER:HB2	2.03	0.41
1:C:432:TYR:O	1:C:520:ARG:HD2	2.21	0.41
1:B:6:LEU:HD12	1:B:45:GLU:HB3	2.02	0.41
1:A:341:LYS:HE2	1:A:345:LYS:HE3	2.03	0.41
1:A:29:GLY:HA2	1:A:498:LYS:O	2.21	0.41
1:A:6:LEU:HD11	1:A:47:ILE:CD1	2.51	0.41
1:A:14[B]:CYS:SG	1:A:417:MET:HB3	2.60	0.41
1:D:14[A]:CYS:SG	1:D:53:PHE:CD2	3.13	0.41
1:B:176:GLN:OE1	1:B:203:GLY:HA3	2.20	0.41
1:D:13:ILE:HD12	1:D:22:ALA:HB3	2.03	0.41
1:C:500:LYS:HD3	4:C:843:HOH:O	2.21	0.41
1:A:92:THR:HG22	1:A:497:VAL:HG22	2.03	0.40
1:B:401:MET:HB2	1:B:402:PRO:HD3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:395:PRO:HD2	1:B:482:PRO:HD3	2.04	0.40
1:A:39:ASP:HA	1:A:40:PRO:HD2	1.98	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	528/559 (94%)	509 (96%)	17 (3%)	2 (0%)	39	56
1	B	528/559 (94%)	512 (97%)	14 (3%)	2 (0%)	39	56
1	C	527/559 (94%)	512 (97%)	13 (2%)	2 (0%)	39	56
1	D	529/559 (95%)	512 (97%)	13 (2%)	4 (1%)	24	35
All	All	2112/2236 (94%)	2045 (97%)	57 (3%)	10 (0%)	39	48

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	172	TYR
1	B	172	TYR
1	C	172	TYR
1	D	172[A]	TYR
1	D	172[B]	TYR
1	D	255	HIS
1	A	396	GLY
1	B	396	GLY
1	D	396	GLY
1	C	396	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	456/479 (95%)	448 (98%)	8 (2%)	66	84
1	B	456/479 (95%)	441 (97%)	15 (3%)	45	66
1	C	455/479 (95%)	443 (97%)	12 (3%)	54	74
1	D	458/479 (96%)	449 (98%)	9 (2%)	63	81
All	All	1825/1916 (95%)	1781 (98%)	44 (2%)	57	76

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	45	GLU
1	A	70	LYS
1	A	120	GLU
1	A	148	GLU
1	A	392	ASN
1	A	476	HIS
1	A	529	LYS
1	A	531	GLU
1	B	45	GLU
1	B	70	LYS
1	B	120	GLU
1	B	148	GLU
1	B	198	LEU
1	B	260	GLN
1	B	292	ARG
1	B	328	TYR
1	B	369	SER
1	B	392	ASN
1	B	404	LEU
1	B	438	LYS
1	B	463	ASN
1	B	476	HIS
1	B	511	GLU
1	C	149	LEU

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Mol	Chain	Res	Type
1	C	202	ASN
1	C	204	ASP
1	C	230	SER
1	C	260	GLN
1	C	304	VAL
1	C	312	SER
1	C	337	GLU
1	C	404	LEU
1	C	419	LYS
1	C	431	VAL
1	C	476	HIS
1	D	32	GLN
1	D	74	ASP
1	D	120	GLU
1	D	260	GLN
1	D	334	ILE
1	D	340	GLN
1	D	404	LEU
1	D	431	VAL
1	D	476	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	260	GLN
1	A	267	GLN
1	A	318	ASN
1	B	260	GLN
1	B	318	ASN
1	C	27	ASN
1	C	202	ASN
1	C	260	GLN
1	C	318	ASN
1	D	260	GLN
1	D	318	ASN
1	D	437	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

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	A	167	1,2	7,11,12	0.64	0	7,12,14	1.64	1 (14%)
1	KCX	B	167	1	7,8,12	0.46	0	6,8,14	0.81	0
1	KCX	C	167	1	7,8,12	0.49	0	6,8,14	0.78	0
1	KCX	D	167	1,2	7,11,12	0.89	1 (14%)	7,12,14	0.96	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	A	167	1,2	-	0/6/10/12	0/0/0/0
1	KCX	B	167	1	-	0/5/7/12	0/0/0/0
1	KCX	C	167	1	-	0/5/7/12	0/0/0/0
1	KCX	D	167	1,2	-	0/6/10/12	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	167	KCX	CE-NZ	2.02	1.50	1.46

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	167	KCX	CE-NZ-CX	-3.67	119.34	123.49

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	167	KCX	1	0
1	B	167	KCX	1	0
1	C	167	KCX	1	0
1	D	167	KCX	1	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 12 ligands modelled in this entry, 8 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	DUC	A	604	2	8,8,8	1.04	1 (12%)	7,10,10	2.60	1 (14%)
3	DUC	B	604	2	8,8,8	1.16	1 (12%)	7,10,10	3.38	1 (14%)
3	DUC	C	604	2	8,8,8	0.77	0	7,10,10	2.97	2 (28%)
3	DUC	D	604	2	8,8,8	0.86	0	7,10,10	3.31	2 (28%)

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	DUC	A	604	2	-	0/0/10/10	0/1/1/1
3	DUC	B	604	2	-	0/0/10/10	0/1/1/1
3	DUC	C	604	2	-	0/0/10/10	0/1/1/1
3	DUC	D	604	2	-	0/0/10/10	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	604	DUC	C4-N3	-2.10	1.34	1.37
3	A	604	DUC	C4-N3	-2.09	1.34	1.37

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	604	DUC	C4-N3-C2	-8.65	118.48	125.75
3	D	604	DUC	C4-N3-C2	-8.07	118.97	125.75
3	C	604	DUC	C4-N3-C2	-7.03	119.84	125.75
3	A	604	DUC	C4-N3-C2	-6.35	120.41	125.75
3	D	604	DUC	O4-C4-N3	2.48	124.33	120.45
3	C	604	DUC	O4-C4-N3	2.74	124.73	120.45

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

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	531/559 (94%)	0.22	20 (3%)	44	45	31, 34, 37, 43	1 (0%)
1	B	531/559 (94%)	0.21	18 (3%)	49	49	31, 34, 37, 43	1 (0%)
1	C	530/559 (94%)	0.30	23 (4%)	39	40	31, 34, 37, 42	0
1	D	531/559 (94%)	0.33	28 (5%)	30	30	31, 34, 37, 43	0
All	All	2123/2236 (94%)	0.26	89 (4%)	40	41	31, 34, 37, 43	2 (0%)

All (89) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	294	HIS	6.8
1	B	294	HIS	6.5
1	C	293	CYS	6.5
1	D	319	PRO	5.4
1	C	303	GLY	5.2
1	D	320	ASP	5.1
1	C	304	VAL	5.0
1	A	293	CYS	4.9
1	D	294	HIS	4.6
1	B	319	PRO	4.4
1	B	293	CYS	4.1
1	C	318	ASN	4.0
1	C	320	ASP	3.9
1	D	542	SER	3.9
1	D	146	ALA	3.8
1	C	316	PHE	3.8
1	D	457	ASP	3.7
1	B	318	ASN	3.7
1	C	457	ASP	3.6
1	D	384	ASN	3.6
1	B	380	GLU	3.6

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Mol	Chain	Res	Type	RSRZ
1	D	315	PRO	3.6
1	A	220	ASP	3.5
1	C	380	GLU	3.4
1	D	318	ASN	3.4
1	A	320	ASP	3.4
1	A	382	ASN	3.4
1	C	319	PRO	3.3
1	C	385	GLY	3.3
1	D	293	CYS	3.3
1	B	320	ASP	3.3
1	C	365	TYR	3.3
1	B	316	PHE	3.2
1	C	324	ILE	3.2
1	A	539	LYS	3.1
1	A	316	PHE	3.1
1	B	322	ARG	3.1
1	A	322	ARG	3.1
1	A	145	GLU	3.0
1	C	323	PHE	2.9
1	C	322	ARG	2.9
1	D	386	GLU	2.9
1	A	149	LEU	2.8
1	D	316	PHE	2.8
1	C	371	ALA	2.7
1	B	303	GLY	2.7
1	D	385	GLY	2.7
1	C	317	THR	2.7
1	C	370	THR	2.7
1	B	382	ASN	2.6
1	D	382	ASN	2.6
1	D	317	THR	2.6
1	B	145	GLU	2.5
1	A	380	GLU	2.5
1	C	328	TYR	2.5
1	D	379	PRO	2.5
1	D	380	GLU	2.5
1	B	304	VAL	2.5
1	B	381	ASN	2.5
1	B	222	TYR	2.4
1	A	463	ASN	2.4
1	C	384	ASN	2.3
1	A	319	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	305	GLY	2.3
1	A	303	GLY	2.3
1	A	148	GLU	2.3
1	D	306	ILE	2.3
1	C	219	THR	2.3
1	D	376	ALA	2.3
1	D	304	VAL	2.3
1	A	318	ASN	2.3
1	D	321	ASP	2.3
1	A	307	ASP	2.2
1	A	540	TYR	2.2
1	D	539	LYS	2.2
1	D	389	TYR	2.2
1	D	365	TYR	2.2
1	B	306	ILE	2.2
1	D	461	GLU	2.2
1	B	541	GLU	2.1
1	D	459	LYS	2.1
1	A	304	VAL	2.1
1	C	310	SER	2.1
1	A	143	SER	2.1
1	B	463	ASN	2.0
1	D	275	VAL	2.0
1	C	382	ASN	2.0
1	B	307	ASP	2.0
1	D	313	GLU	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. 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, 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	LLDF	B-factors(Å^2)	Q<0.9
1	KCX	D	167	12/13	0.83	0.20	-	33,35,45,46	3
1	KCX	B	167	9/13	0.95	0.18	-	34,34,38,39	0
1	KCX	C	167	9/13	0.94	0.18	-	33,34,37,37	0
1	KCX	A	167	12/13	0.75	0.24	-	33,34,46,46	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. 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, 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	LLDF	B-factors(Å^2)	Q<0.9
2	ZN	D	602	1/1	0.83	0.44	16.50	51,51,51,51	1
2	ZN	B	602	1/1	0.28	0.46	12.22	53,53,53,53	1
2	ZN	A	602	1/1	0.96	0.38	9.81	49,49,49,49	1
2	ZN	C	602	1/1	0.90	0.32	5.82	50,50,50,50	1
3	DUC	A	604	8/8	0.85	0.26	3.99	52,55,56,56	0
3	DUC	D	604	8/8	0.83	0.26	3.40	52,55,57,57	0
3	DUC	B	604	8/8	0.86	0.24	3.03	56,59,59,59	0
3	DUC	C	604	8/8	0.76	0.22	1.28	55,59,59,60	0
2	ZN	D	601	1/1	0.95	0.19	-	47,47,47,47	0
2	ZN	A	601	1/1	0.97	0.23	-	46,46,46,46	0
2	ZN	B	601	1/1	0.95	0.15	-	45,45,45,45	0
2	ZN	C	601	1/1	0.97	0.17	-	44,44,44,44	1

6.5 Other polymers (i)

There are no such residues in this entry.