



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 04:47 PM GMT

PDB ID : 4G7E  
Title : Crystal structure of pigeon pea urease  
Authors : Balasubramanian, A.; Ponnuraj, K.  
Deposited on : 2012-07-20  
Resolution : 2.20 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](mailto: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.

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The following versions of software and data (see [references ⓘ](#)) 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

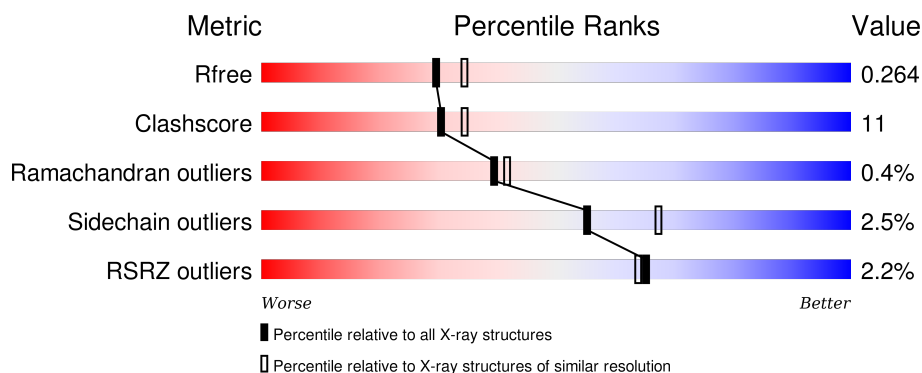
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*



The reported resolution of this entry is 2.20 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	3774 (2.20-2.20)
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (2.20-2.20)

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  $\geq 3$ , 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	840	 3% 79% 18% ..
2	B	840	 2% 81% 16% ..

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 13171 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 urease.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	833	Total	C	N	O	S	0	0	0
			6254	3933	1080	1204	37			

- Molecule 2 is a protein called urease.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	833	Total	C	N	O	S	0	0	0
			6256	3933	1080	1205	38			

- Molecule 3 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	2	Total	Ni	0	0
			2	2		
3	A	2	Total	Ni	0	0
			2	2		

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

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

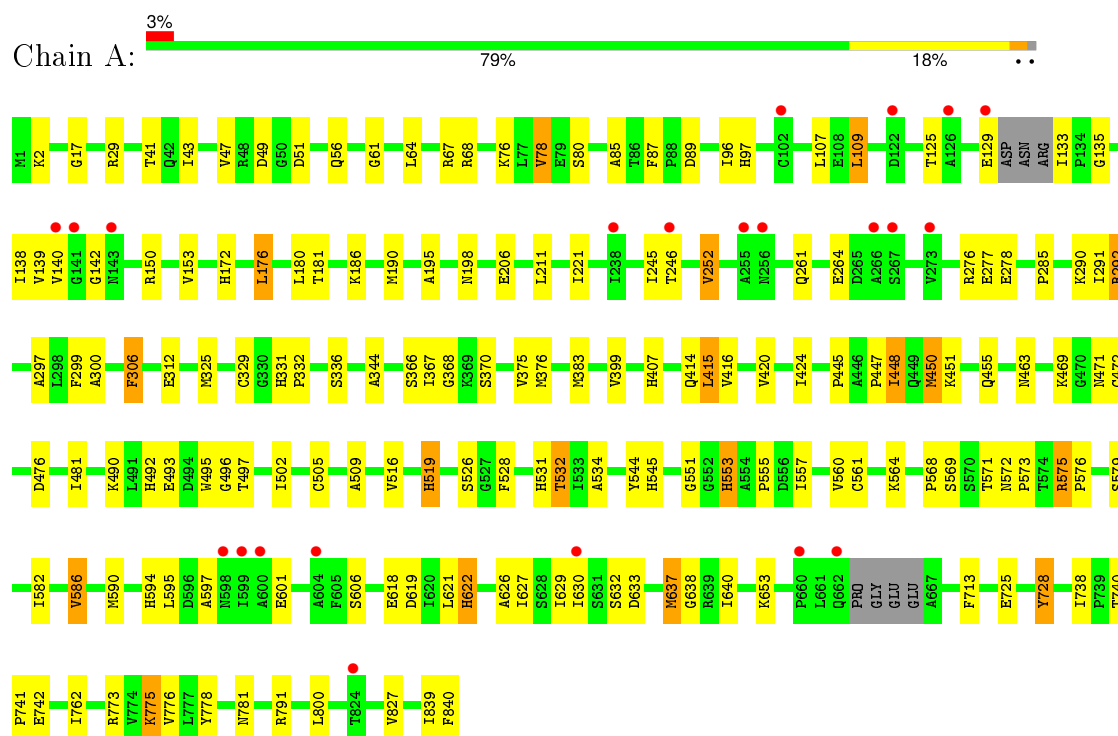
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	299	Total	O	0	0
			299	299		
5	B	357	Total	O	0	0
			357	357		

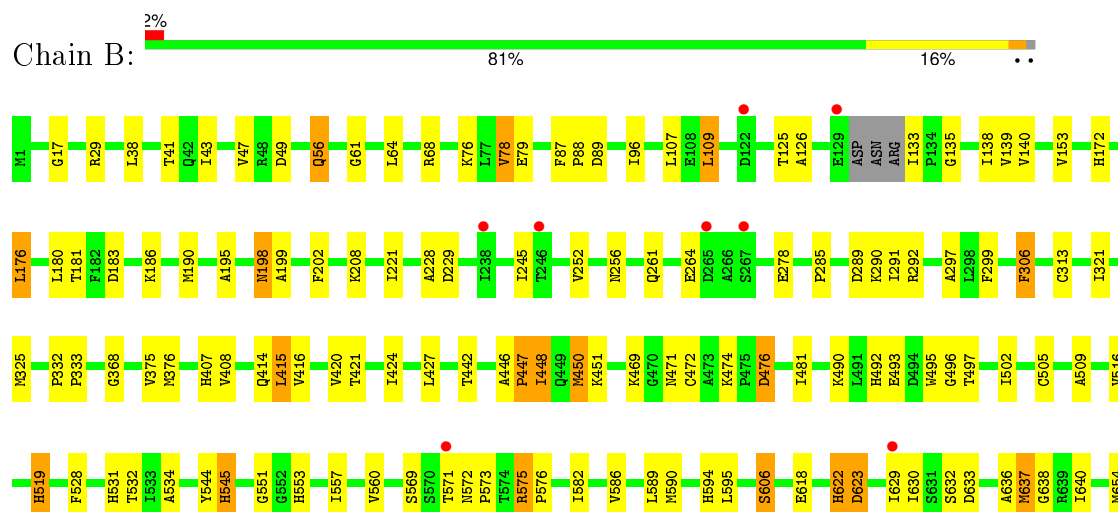
### 3 Residue-property plots

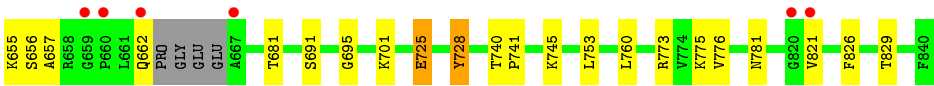
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: urease



#### • Molecule 2: urease





## 4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	176.29Å 176.29Å 346.44Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.70 – 2.20 29.70 – 2.20	Depositor EDS
% Data completeness (in resolution range)	98.8 (29.70-2.20) 98.8 (29.70-2.20)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.07 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.0	Depositor
R, $R_{free}$	0.217 , 0.268 0.216 , 0.264	Depositor DCC
$R_{free}$ test set	5232 reflections (5.32%)	DCC
Wilson B-factor (Å <sup>2</sup> )	34.4	Xtriage
Anisotropy	0.051	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 36.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.53$ , $\langle L^2 \rangle = 0.37$	Xtriage
Outliers	5 of 103449 reflections (0.005%)	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	13171	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.76% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  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: NI, CME, MG, 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	0.91	7/6340 (0.1%)	0.91	10/8597 (0.1%)
2	B	0.89	7/6331 (0.1%)	0.89	11/8584 (0.1%)
All	All	0.90	14/12671 (0.1%)	0.90	21/17181 (0.1%)

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	472	CYS	CB-SG	-10.54	1.64	1.82
1	A	329	CYS	CB-SG	-8.32	1.68	1.82
2	B	472	CYS	CB-SG	-7.67	1.69	1.82
2	B	505	CYS	CB-SG	-7.29	1.69	1.82
2	B	493	GLU	CD-OE2	-6.61	1.18	1.25
1	A	505	CYS	CB-SG	-6.58	1.71	1.82
2	B	493	GLU	CD-OE1	-5.70	1.19	1.25
2	B	198	ASN	CB-CG	-5.63	1.38	1.51
1	A	306	PHE	CE1-CZ	-5.57	1.26	1.37
2	B	725	GLU	CB-CG	-5.53	1.41	1.52
1	A	725	GLU	CG-CD	-5.39	1.43	1.51
1	A	742	GLU	CD-OE1	-5.38	1.19	1.25
1	A	725	GLU	CB-CG	-5.14	1.42	1.52
2	B	306	PHE	CE2-CZ	-5.00	1.27	1.37

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	575	ARG	NE-CZ-NH1	9.59	125.09	120.30
2	B	176	LEU	CB-CG-CD2	-9.27	95.25	111.00
1	A	176	LEU	CB-CG-CD2	-8.99	95.71	111.00
2	B	493	GLU	OE1-CD-OE2	-7.25	114.59	123.30
2	B	575	ARG	NE-CZ-NH2	6.89	123.74	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	89	ASP	CB-CG-OD2	6.61	124.25	118.30
1	A	742	GLU	OE1-CD-OE2	-6.48	115.52	123.30
2	B	623	ASP	CB-CG-OD1	6.22	123.89	118.30
1	A	526	SER	N-CA-CB	-6.17	101.24	110.50
2	B	109	LEU	CB-CG-CD2	-6.04	100.74	111.00
2	B	476	ASP	CB-CG-OD1	5.99	123.69	118.30
2	B	278	GLU	CG-CD-OE1	-5.95	106.41	118.30
1	A	292	ARG	NE-CZ-NH2	5.89	123.25	120.30
2	B	49	ASP	CB-CG-OD2	5.84	123.56	118.30
1	A	109	LEU	CB-CG-CD2	-5.59	101.49	111.00
1	A	312	GLU	OE1-CD-OE2	-5.58	116.60	123.30
2	B	261	GLN	CB-CA-C	-5.31	99.79	110.40
1	A	450	MET	CB-CG-SD	-5.23	96.72	112.40
1	A	493	GLU	OE1-CD-OE2	-5.20	117.06	123.30
1	A	89	ASP	CB-CG-OD2	5.06	122.86	118.30
2	B	450	MET	CB-CG-SD	-5.03	97.30	112.40

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	6254	0	6269	138	0
2	B	6256	0	6267	141	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
4	B	1	0	0	0	0
5	A	299	0	0	19	0
5	B	357	0	0	29	0
All	All	13171	0	12536	276	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 11.

All (276) 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:471:ASN:OD1	1:A:496:GLY:O	1.66	1.14
2:B:474:LYS:HE3	5:B:1345:HOH:O	1.46	1.11
1:A:211:LEU:HD22	5:A:1275:HOH:O	1.51	1.07
1:A:573:PRO:HG3	1:A:637:MET:O	1.54	1.06
1:A:245:ILE:HG13	5:A:1147:HOH:O	1.58	1.01
1:A:246:THR:HG21	5:A:1274:HOH:O	1.61	1.01
2:B:662:GLN:HG3	5:B:1320:HOH:O	1.59	0.98
1:A:528:PHE:H	1:A:531:HIS:CD2	1.84	0.96
2:B:528:PHE:H	2:B:531:HIS:HD2	1.07	0.95
1:A:450:MET:HE1	1:A:481:ILE:HD11	1.47	0.95
2:B:450:MET:CE	2:B:481:ILE:HD11	1.98	0.93
1:A:448:ILE:H	1:A:448:ILE:HD12	1.33	0.92
1:A:51:ASP:HB2	5:A:1293:HOH:O	1.69	0.92
1:A:43:ILE:O	1:A:47:VAL:HG23	1.70	0.92
1:A:450:MET:CE	1:A:481:ILE:HD11	1.99	0.92
1:A:528:PHE:H	1:A:531:HIS:HD2	0.95	0.90
1:A:471:ASN:HD21	1:A:492:HIS:H	1.19	0.89
2:B:252:VAL:HG21	5:B:1336:HOH:O	1.73	0.89
2:B:448:ILE:H	2:B:448:ILE:HD12	1.38	0.88
1:A:172:HIS:CD2	1:A:221:ILE:HG12	2.09	0.87
2:B:450:MET:HE1	2:B:481:ILE:HD11	1.56	0.87
2:B:573:PRO:HG3	2:B:637:MET:O	1.75	0.86
2:B:448:ILE:HG13	5:B:1357:HOH:O	1.75	0.85
1:A:528:PHE:N	1:A:531:HIS:HD2	1.74	0.85
1:A:172:HIS:HD2	1:A:221:ILE:HG12	1.41	0.84
1:A:64:LEU:CD2	1:A:109:LEU:HD23	2.06	0.83
2:B:442:THR:OG1	2:B:490:KCX:HG2	1.80	0.81
1:A:448:ILE:CD1	1:A:448:ILE:H	1.94	0.80
2:B:471:ASN:ND2	2:B:496:GLY:O	2.16	0.79
2:B:43:ILE:O	2:B:47:VAL:HG23	1.82	0.79
1:A:532:THR:HG21	5:A:1176:HOH:O	1.82	0.79
2:B:256:ASN:HB2	5:B:1114:HOH:O	1.82	0.79
1:A:582:ILE:O	1:A:586:VAL:HG23	1.82	0.78
2:B:528:PHE:H	2:B:531:HIS:CD2	1.97	0.78
2:B:471:ASN:OD1	2:B:495:TRP:HB2	1.85	0.77
2:B:415:LEU:HD12	2:B:640:ILE:HG12	1.66	0.77
2:B:245:ILE:HG13	5:B:1291:HOH:O	1.84	0.76
2:B:528:PHE:N	2:B:531:HIS:HD2	1.82	0.76
1:A:415:LEU:HD12	1:A:640:ILE:HG12	1.66	0.76
1:A:64:LEU:HD23	1:A:109:LEU:CD2	2.15	0.75
2:B:448:ILE:H	2:B:448:ILE:CD1	2.00	0.74
1:A:181:THR:HG22	1:A:252:VAL:HG23	1.69	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:367:ILE:C	1:A:383:MET:HE1	2.07	0.74
2:B:64:LEU:CD2	2:B:109:LEU:HD23	2.19	0.73
2:B:502:ILE:CD1	2:B:532:THR:HG23	2.18	0.72
2:B:582:ILE:O	2:B:586:VAL:HG23	1.88	0.72
2:B:79:GLU:HA	2:B:79:GLU:OE1	1.88	0.72
1:A:502:ILE:CD1	1:A:532:THR:HG22	2.20	0.71
2:B:534:ALA:HB1	5:B:1306:HOH:O	1.90	0.71
1:A:64:LEU:HD23	1:A:109:LEU:HD23	1.71	0.70
1:A:532:THR:OG1	1:A:553:HIS:NE2	2.24	0.70
2:B:775:LYS:HG3	5:B:1352:HOH:O	1.91	0.70
2:B:590:MET:HE1	2:B:595:LEU:HD12	1.73	0.70
2:B:195:ALA:HB3	2:B:198:ASN:HD21	1.57	0.70
1:A:176:LEU:HD23	1:A:180:LEU:HD12	1.73	0.69
2:B:469:LYS:HE2	2:B:495:TRP:CE2	2.28	0.69
2:B:306:PHE:CD2	2:B:368:GLY:HA2	2.28	0.69
2:B:415:LEU:HG	2:B:416:VAL:N	2.08	0.68
1:A:195:ALA:HB3	1:A:198:ASN:HD21	1.58	0.68
1:A:64:LEU:CD2	1:A:109:LEU:CD2	2.72	0.68
2:B:172:HIS:CD2	2:B:221:ILE:HG23	2.30	0.67
1:A:407:HIS:CE1	1:A:544:TYR:CD2	2.83	0.66
2:B:64:LEU:CD2	2:B:109:LEU:CD2	2.73	0.66
2:B:590:MET:CE	2:B:595:LEU:HD12	2.26	0.65
1:A:61:GLY:HA3	1:A:96:ILE:HG12	1.79	0.65
2:B:415:LEU:CD1	2:B:640:ILE:HD13	2.27	0.64
2:B:140:VAL:HG21	5:B:1304:HOH:O	1.97	0.64
1:A:366:SER:HB2	1:A:383:MET:HE2	1.79	0.64
2:B:375:VAL:HG23	2:B:376:MET:HG3	1.78	0.64
2:B:773:ARG:HA	2:B:775:LYS:HE2	1.80	0.64
2:B:632:SER:O	2:B:638:GLY:HA3	1.99	0.63
2:B:415:LEU:HD13	2:B:640:ILE:HD13	1.80	0.63
2:B:126:ALA:CB	5:B:1330:HOH:O	2.46	0.63
1:A:773:ARG:HB3	1:A:775:LYS:HE2	1.81	0.63
1:A:368:GLY:HA3	1:A:383:MET:HE3	1.81	0.62
1:A:450:MET:CE	1:A:481:ILE:CD1	2.77	0.62
1:A:415:LEU:HG	1:A:416:VAL:N	2.15	0.61
1:A:632:SER:O	1:A:638:GLY:HA3	2.00	0.61
1:A:492:HIS:C	1:A:497:THR:HG23	2.20	0.61
1:A:325:MET:O	1:A:375:VAL:HG21	2.00	0.60
2:B:775:LYS:CG	5:B:1352:HOH:O	2.49	0.60
1:A:285:PRO:HG3	1:A:291:ILE:HD11	1.83	0.60
1:A:622:HIS:CE1	1:A:630:ILE:HG13	2.37	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:450:MET:HE1	1:A:481:ILE:CD1	2.28	0.59
1:A:211:LEU:CD2	5:A:1275:HOH:O	2.26	0.59
2:B:64:LEU:HD23	2:B:109:LEU:CD2	2.32	0.59
1:A:415:LEU:HD12	1:A:640:ILE:CG1	2.31	0.59
2:B:745:LYS:HE3	5:B:1193:HOH:O	2.01	0.59
2:B:290:LYS:HE3	5:B:1091:HOH:O	2.03	0.59
2:B:285:PRO:HG3	2:B:291:ILE:HD11	1.84	0.59
2:B:450:MET:CE	2:B:481:ILE:CD1	2.78	0.58
1:A:181:THR:CG2	1:A:252:VAL:HG23	2.32	0.58
1:A:176:LEU:CD2	1:A:180:LEU:HD12	2.33	0.58
2:B:139:VAL:HB	5:B:1309:HOH:O	2.03	0.58
1:A:597:ALA:HB2	5:A:1298:HOH:O	2.02	0.58
1:A:469:LYS:HE2	1:A:495:TRP:CE2	2.38	0.58
2:B:448:ILE:CG1	5:B:1357:HOH:O	2.44	0.57
2:B:469:LYS:HE2	2:B:495:TRP:CD2	2.40	0.57
1:A:367:ILE:N	1:A:383:MET:HE1	2.19	0.57
1:A:415:LEU:CD1	1:A:640:ILE:HD13	2.35	0.57
2:B:492:HIS:C	2:B:497:THR:HG23	2.24	0.57
2:B:618:GLU:O	2:B:622:HIS:HB2	2.05	0.56
2:B:325:MET:O	2:B:375:VAL:HG21	2.04	0.56
2:B:590:MET:HE1	2:B:595:LEU:CD1	2.34	0.56
1:A:781:ASN:HB3	5:A:1284:HOH:O	2.04	0.56
2:B:61:GLY:HA3	2:B:96:ILE:HG12	1.88	0.56
1:A:76:LYS:HE2	1:A:133:ILE:HG12	1.86	0.56
1:A:78:VAL:O	1:A:78:VAL:HG13	2.06	0.56
2:B:153:VAL:HG12	2:B:190:MET:HE2	1.87	0.55
2:B:622:HIS:HE1	2:B:630:ILE:HG13	1.71	0.55
1:A:773:ARG:CB	1:A:775:LYS:HE2	2.36	0.55
2:B:420:VAL:HA	2:B:424:ILE:O	2.06	0.55
1:A:367:ILE:C	1:A:383:MET:CE	2.74	0.55
1:A:564:LYS:HE2	5:A:1182:HOH:O	2.07	0.55
1:A:246:THR:CG2	5:A:1274:HOH:O	2.35	0.55
2:B:775:LYS:HD2	5:B:1352:HOH:O	2.06	0.55
2:B:297:ALA:HB3	5:B:1326:HOH:O	2.07	0.55
1:A:509:ALA:O	1:A:791:ARG:HD3	2.07	0.55
1:A:420:VAL:HA	1:A:424:ILE:O	2.07	0.55
2:B:183:ASP:OD2	2:B:186:LYS:HD2	2.07	0.54
2:B:821:VAL:HG21	5:B:1277:HOH:O	2.07	0.54
2:B:622:HIS:CE1	2:B:630:ILE:HG13	2.43	0.54
2:B:589:LEU:HD23	2:B:606:SER:HB2	1.89	0.54
2:B:557:ILE:O	2:B:560:VAL:HG22	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:264:GLU:O	2:B:264:GLU:HG2	2.07	0.54
2:B:415:LEU:CD1	2:B:640:ILE:CD1	2.86	0.54
1:A:142:GLY:O	1:A:276:ARG:HB2	2.08	0.54
2:B:451:LYS:HD3	5:B:1335:HOH:O	2.08	0.54
2:B:181:THR:CG2	2:B:252:VAL:HG23	2.38	0.53
2:B:829:THR:HG22	5:B:1174:HOH:O	2.08	0.53
2:B:590:MET:HE1	2:B:595:LEU:HB2	1.90	0.53
1:A:375:VAL:HG23	1:A:376:MET:HG3	1.89	0.53
2:B:622:HIS:CE1	2:B:630:ILE:CG1	2.92	0.53
1:A:502:ILE:HD12	1:A:532:THR:HG22	1.91	0.52
2:B:313:CYS:HB3	2:B:321:ILE:HD11	1.91	0.52
2:B:126:ALA:HB2	5:B:1330:HOH:O	2.09	0.52
1:A:344:ALA:HB1	1:A:399:VAL:HG23	1.92	0.52
1:A:332:PRO:HB3	2:B:476:ASP:OD1	2.09	0.52
2:B:421:THR:HG22	2:B:728:TYR:CE1	2.45	0.52
1:A:331:HIS:HE2	1:A:336:SER:HG	1.54	0.52
1:A:463:ASN:HA	1:A:762:ILE:O	2.08	0.52
2:B:594:HIS:CE1	5:B:1286:HOH:O	2.61	0.52
1:A:773:ARG:HA	1:A:775:LYS:HE2	1.91	0.52
1:A:150:ARG:O	1:A:261:GLN:HB2	2.10	0.51
1:A:206:GLU:HG3	5:A:1283:HOH:O	2.09	0.51
2:B:636:ALA:O	2:B:637:MET:HB2	2.10	0.51
2:B:78:VAL:HG13	2:B:78:VAL:O	2.11	0.51
2:B:202:PHE:HE1	2:B:208:LYS:HB2	1.76	0.50
1:A:366:SER:HB2	1:A:383:MET:CE	2.41	0.50
2:B:202:PHE:CE1	2:B:208:LYS:HB2	2.46	0.50
2:B:534:ALA:CB	5:B:1306:HOH:O	2.55	0.50
1:A:140:VAL:O	1:A:276:ARG:HG2	2.12	0.50
1:A:80:SER:HB3	1:A:97:HIS:HA	1.92	0.50
1:A:590:MET:HE1	1:A:595:LEU:HB2	1.93	0.50
1:A:153:VAL:HG12	1:A:190:MET:HE2	1.93	0.50
1:A:839:ILE:O	1:A:839:ILE:HG13	2.12	0.50
2:B:415:LEU:HD12	2:B:640:ILE:CG1	2.38	0.50
2:B:691:SER:O	2:B:701:LYS:HE2	2.11	0.50
2:B:76:LYS:HE2	2:B:133:ILE:HG12	1.93	0.49
2:B:740:THR:N	2:B:741:PRO:CD	2.75	0.49
2:B:775:LYS:HG2	2:B:776:VAL:H	1.77	0.49
2:B:775:LYS:CD	5:B:1352:HOH:O	2.60	0.49
2:B:198:ASN:HB2	5:B:1075:HOH:O	2.12	0.49
1:A:297:ALA:HB2	5:A:1217:HOH:O	2.12	0.49
1:A:138:ILE:HD12	1:A:299:PHE:CE2	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:135:GLY:HA2	2:B:292:ARG:O	2.13	0.49
2:B:176:LEU:HD23	2:B:180:LEU:HD12	1.95	0.49
2:B:29:ARG:NH1	2:B:68:ARG:O	2.46	0.49
2:B:138:ILE:HD12	2:B:299:PHE:CE2	2.48	0.48
1:A:176:LEU:HD23	1:A:180:LEU:CD1	2.43	0.48
1:A:622:HIS:HE1	1:A:630:ILE:HG13	1.77	0.48
2:B:407:HIS:CE1	2:B:544:TYR:CD2	3.01	0.48
2:B:569:SER:HB3	2:B:629:ILE:HB	1.95	0.48
1:A:186:LYS:HE2	5:A:1035:HOH:O	2.14	0.48
2:B:775:LYS:HE3	2:B:776:VAL:HG23	1.96	0.48
1:A:775:LYS:HE3	1:A:776:VAL:HG23	1.96	0.47
1:A:557:ILE:O	1:A:560:VAL:HG22	2.13	0.47
1:A:519:HIS:CE1	1:A:551:GLY:HA3	2.49	0.47
1:A:129:GLU:C	5:A:1288:HOH:O	2.53	0.47
1:A:575:ARG:HA	1:A:576:PRO:HA	1.79	0.47
1:A:594:HIS:CE1	5:A:1049:HOH:O	2.67	0.47
1:A:17:GLY:HA3	1:A:41:THR:OG1	2.15	0.46
1:A:740:THR:N	1:A:741:PRO:CD	2.78	0.46
1:A:445:PRO:O	1:A:481:ILE:HD13	2.15	0.46
2:B:775:LYS:CG	2:B:776:VAL:N	2.78	0.46
2:B:509:ALA:HB2	2:B:516:VAL:HG23	1.98	0.46
2:B:781:ASN:HB3	5:B:1319:HOH:O	2.16	0.46
1:A:325:MET:O	1:A:375:VAL:CG2	2.63	0.46
2:B:775:LYS:HG2	2:B:776:VAL:N	2.30	0.46
2:B:450:MET:HE3	2:B:481:ILE:CD1	2.46	0.46
1:A:569:SER:HB3	1:A:629:ILE:HB	1.98	0.46
2:B:47:VAL:HG22	2:B:87:PHE:CZ	2.51	0.45
2:B:773:ARG:HE	2:B:775:LYS:HZ1	1.64	0.45
2:B:725:GLU:HG2	2:B:760:LEU:HD11	1.98	0.45
1:A:618:GLU:O	1:A:622:HIS:HB2	2.15	0.45
2:B:622:HIS:CE1	2:B:630:ILE:HD11	2.51	0.45
1:A:590:MET:HE3	1:A:606:SER:CB	2.47	0.45
2:B:292:ARG:HG3	2:B:292:ARG:HH11	1.81	0.45
1:A:306:PHE:CD2	1:A:368:GLY:HA2	2.51	0.45
1:A:469:LYS:HE2	1:A:495:TRP:CD2	2.52	0.45
2:B:572:ASN:N	2:B:573:PRO:CD	2.80	0.45
1:A:47:VAL:HG21	1:A:85:ALA:HB3	1.98	0.45
1:A:579:SER:HA	1:A:827:VAL:CG1	2.47	0.45
2:B:321:ILE:HG22	2:B:321:ILE:O	2.16	0.44
2:B:17:GLY:HA3	2:B:41:THR:OG1	2.18	0.44
1:A:47:VAL:HG13	1:A:87:PHE:CG	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:622:HIS:CE1	1:A:630:ILE:CG1	3.00	0.44
2:B:38:LEU:HD23	2:B:38:LEU:C	2.37	0.44
1:A:135:GLY:HA2	1:A:292:ARG:O	2.18	0.44
1:A:29:ARG:NH2	1:A:67:ARG:HH12	2.15	0.44
1:A:471:ASN:ND2	1:A:492:HIS:H	1.99	0.44
1:A:839:ILE:HG23	1:A:840:PHE:CD2	2.53	0.44
2:B:502:ILE:CD1	2:B:532:THR:CG2	2.92	0.43
1:A:43:ILE:HG13	1:A:96:ILE:HD11	2.00	0.43
1:A:181:THR:CG2	1:A:252:VAL:CG2	2.96	0.43
1:A:451:LYS:O	1:A:455:GLN:HG3	2.18	0.43
1:A:590:MET:CE	1:A:595:LEU:HD12	2.48	0.43
2:B:519:HIS:CE1	2:B:551:GLY:HA3	2.53	0.43
2:B:64:LEU:HD23	2:B:109:LEU:HD22	2.01	0.43
2:B:740:THR:N	2:B:741:PRO:HD3	2.34	0.43
2:B:657:ALA:HB2	2:B:826:PHE:HE2	1.83	0.43
1:A:572:ASN:N	1:A:573:PRO:CD	2.81	0.43
2:B:252:VAL:HG11	5:B:1336:HOH:O	2.18	0.43
2:B:502:ILE:HD13	2:B:532:THR:HG23	1.97	0.43
2:B:446:ALA:HB1	2:B:448:ILE:HD13	2.01	0.43
2:B:47:VAL:HG13	2:B:87:PHE:CG	2.53	0.43
2:B:681:THR:HB	2:B:695:GLY:O	2.19	0.42
2:B:575:ARG:HA	2:B:576:PRO:HA	1.82	0.42
1:A:571:THR:CG2	1:A:633:ASP:HB2	2.49	0.42
1:A:561:CYS:SG	1:A:627:ILE:HG12	2.58	0.42
1:A:532:THR:HG23	5:A:1155:HOH:O	2.17	0.42
2:B:502:ILE:HD11	2:B:532:THR:HG23	2.00	0.42
2:B:139:VAL:HG12	2:B:140:VAL:O	2.19	0.42
1:A:29:ARG:HH22	1:A:67:ARG:HH12	1.66	0.42
1:A:415:LEU:CD1	1:A:640:ILE:CD1	2.98	0.42
1:A:2:LYS:HB3	1:A:2:LYS:HE3	1.90	0.42
2:B:285:PRO:HB2	2:B:289:ASP:HB2	2.02	0.42
1:A:29:ARG:NH1	1:A:68:ARG:O	2.53	0.42
2:B:228:ALA:O	2:B:229:ASP:C	2.58	0.42
2:B:623:ASP:HB2	2:B:654:MET:HG3	2.01	0.42
1:A:773:ARG:CA	1:A:775:LYS:HE2	2.50	0.42
1:A:332:PRO:HB3	2:B:476:ASP:HA	2.00	0.42
1:A:471:ASN:ND2	1:A:495:TRP:HB2	2.35	0.42
2:B:447:PRO:HB2	2:B:448:ILE:HD12	2.02	0.42
2:B:571:THR:CG2	2:B:633:ASP:HB2	2.50	0.42
1:A:509:ALA:HB2	1:A:516:VAL:HG23	2.01	0.41
1:A:713:PHE:CD1	1:A:713:PHE:C	2.93	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:264:GLU:O	1:A:264:GLU:HG2	2.19	0.41
2:B:655:LYS:HD3	5:B:1326:HOH:O	2.19	0.41
1:A:621:LEU:HB3	1:A:626:ALA:HB3	2.02	0.41
2:B:198:ASN:HB2	2:B:199:ALA:H	1.67	0.41
2:B:408:VAL:HG21	2:B:427:LEU:HB3	2.01	0.41
1:A:290:LYS:HA	1:A:300:ALA:O	2.21	0.41
1:A:139:VAL:HG21	1:A:277:GLU:HA	2.02	0.41
1:A:728:TYR:HE2	5:A:1137:HOH:O	2.03	0.41
1:A:78:VAL:O	1:A:78:VAL:CG1	2.67	0.41
1:A:490:KCX:CX	1:A:492:HIS:HD2	2.34	0.41
2:B:544:TYR:O	2:B:545:HIS:C	2.58	0.41
1:A:534:ALA:CB	5:A:1139:HOH:O	2.69	0.41
1:A:245:ILE:CD1	5:A:1147:HOH:O	2.69	0.41
2:B:78:VAL:CG1	2:B:78:VAL:O	2.67	0.41
1:A:292:ARG:NH1	1:A:299:PHE:CZ	2.89	0.41
1:A:476:ASP:HA	2:B:332:PRO:HB3	2.03	0.41
2:B:56:GLN:HG2	5:B:1029:HOH:O	2.21	0.41
1:A:447:PRO:HB2	1:A:448:ILE:HD12	2.02	0.41
2:B:87:PHE:HB3	2:B:88:PRO:CD	2.51	0.41
2:B:590:MET:HE1	2:B:595:LEU:CB	2.50	0.41
2:B:47:VAL:HG13	2:B:87:PHE:CD1	2.56	0.41
2:B:502:ILE:HD13	2:B:532:THR:CG2	2.51	0.41
1:A:451:LYS:HG3	1:A:778:TYR:CD2	2.56	0.41
1:A:586:VAL:O	1:A:590:MET:HG2	2.20	0.40
2:B:332:PRO:HA	2:B:333:PRO:HD3	1.94	0.40
2:B:87:PHE:HB3	2:B:88:PRO:HD2	2.03	0.40
1:A:278:GLU:HA	1:A:278:GLU:OE1	2.21	0.40
1:A:738:ILE:HG13	1:A:741:PRO:HD3	2.03	0.40
1:A:619:ASP:OD2	1:A:653:LYS:NZ	2.44	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	825/840 (98%)	782 (95%)	39 (5%)	4 (0%)	34	35
2	B	824/840 (98%)	779 (94%)	42 (5%)	3 (0%)	39	42
All	All	1649/1680 (98%)	1561 (95%)	81 (5%)	7 (0%)	39	42

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	637	MET
1	A	545	HIS
1	A	553	HIS
1	A	637	MET
2	B	545	HIS
2	B	553	HIS
1	A	568	PRO

### 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	666/672 (99%)	647 (97%)	19 (3%)	50	62
2	B	665/671 (99%)	651 (98%)	14 (2%)	61	74
All	All	1331/1343 (99%)	1298 (98%)	33 (2%)	55	67

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	49	ASP
1	A	56	GLN
1	A	78	VAL
1	A	107	LEU
1	A	125	THR
1	A	252	VAL
1	A	370	SER
1	A	414	GLN
1	A	415	LEU

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Mol	Chain	Res	Type
1	A	448	ILE
1	A	519	HIS
1	A	532	THR
1	A	555	PRO
1	A	586	VAL
1	A	601	GLU
1	A	622	HIS
1	A	728	TYR
1	A	775	LYS
1	A	800	LEU
2	B	56	GLN
2	B	78	VAL
2	B	107	LEU
2	B	125	THR
2	B	414	GLN
2	B	415	LEU
2	B	447	PRO
2	B	448	ILE
2	B	519	HIS
2	B	606	SER
2	B	622	HIS
2	B	656	SER
2	B	728	TYR
2	B	753	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	82	GLN
1	A	172	HIS
1	A	198	ASN
1	A	455	GLN
1	A	471	ASN
1	A	531	HIS
1	A	649	GLN
2	B	82	GLN
2	B	198	ASN
2	B	531	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

5 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	490	1,3	7,11,12	0.79	0	7,12,14	1.43	1 (14%)
1	CME	A	592	1	8,9,10	0.72	0	6,9,11	2.59	2 (33%)
2	CME	B	207	2	8,9,10	0.79	0	6,9,11	1.69	2 (33%)
2	KCX	B	490	3,2	7,11,12	1.15	0	7,12,14	1.39	1 (14%)
2	CME	B	592	2	8,9,10	0.64	0	6,9,11	1.78	2 (33%)

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	490	1,3	-	0/6/10/12	0/0/0/0
1	CME	A	592	1	-	0/5/8/10	0/0/0/0
2	CME	B	207	2	-	0/5/8/10	0/0/0/0
2	KCX	B	490	3,2	-	0/6/10/12	0/0/0/0
2	CME	B	592	2	-	0/5/8/10	0/0/0/0

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	592	CME	CB-SG-SD	-5.46	93.31	103.95
2	B	592	CME	CB-SG-SD	-3.56	97.01	103.95
1	A	490	KCX	CE-NZ-CX	-2.89	120.22	123.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	592	CME	O-C-CA	-2.68	118.52	125.49
2	B	207	CME	CB-SG-SD	-2.22	99.62	103.95
2	B	592	CME	O-C-CA	-2.09	120.06	125.49
2	B	207	CME	CE-SD-SG	2.54	116.71	103.56
2	B	490	KCX	CE-NZ-CX	2.69	126.54	123.49

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	490	KCX	1	0
2	B	490	KCX	1	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 5 are monoatomic - leaving 0 for Mogul analysis.

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.

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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	831/840 (98%)	-0.26	22 (2%) 59 58	21, 32, 47, 72	0
2	B	830/840 (98%)	-0.31	14 (1%) 73 72	22, 32, 47, 72	0
All	All	1661/1680 (98%)	-0.29	36 (2%) 65 64	21, 32, 47, 72	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	662	GLN	4.6
1	A	598	ASN	4.3
1	A	599	ILE	3.8
1	A	256	ASN	3.7
1	A	267	SER	3.6
1	A	140	VAL	3.4
2	B	238	ILE	3.2
2	B	662	GLN	3.2
1	A	604	ALA	3.1
1	A	122	ASP	3.1
1	A	246	THR	3.0
1	A	141	GLY	3.0
2	B	659	GLY	2.9
2	B	820	GLY	2.9
1	A	660	PRO	2.8
1	A	102	CYS	2.8
1	A	238	ILE	2.7
1	A	266	ALA	2.6
2	B	265	ASP	2.5
2	B	267	SER	2.5
2	B	821	VAL	2.5
2	B	629	ILE	2.5
2	B	129	GLU	2.5
1	A	273	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	129	GLU	2.3
1	A	630	ILE	2.2
1	A	255	ALA	2.2
1	A	824	THR	2.2
1	A	143	ASN	2.2
2	B	660	PRO	2.1
2	B	571	THR	2.1
1	A	600	ALA	2.1
2	B	667	ALA	2.1
1	A	126	ALA	2.1
2	B	122	ASP	2.1
2	B	246	THR	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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	KCX	A	490	12/13	0.95	0.11	-	19,22,24,24	0
1	CME	A	592	10/11	0.94	0.12	-	39,40,41,42	0
2	CME	B	592	10/11	0.98	0.06	-	39,40,40,41	0
2	CME	B	207	10/11	0.98	0.12	-	38,41,47,48	0
2	KCX	B	490	12/13	0.97	0.11	-	18,21,23,24	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<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
3	NI	B	901	1/1	1.00	0.08	-1.07	33,33,33,33	0
4	MG	B	903	1/1	0.99	0.05	-1.56	32,32,32,32	0
3	NI	A	901	1/1	0.99	0.05	-2.57	40,40,40,40	0
3	NI	A	902	1/1	0.99	0.03	-2.74	34,34,34,34	0
3	NI	B	902	1/1	0.99	0.05	-2.98	37,37,37,37	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.