



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 11:22 AM GMT

PDB ID : 3OS8  
Title : Estrogen Receptor  
Authors : Bruning, J.; Parent, A.A.; Gil, G.; Zhao, M.; Nowak, J.; Pace, M.C.; Smith, C.L.; Afonine, P.V.; Adams, P.D.; Katzenellenbogen, J.A.; Nettles, K.W.  
Deposited on : 2010-09-08  
Resolution : 2.03 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

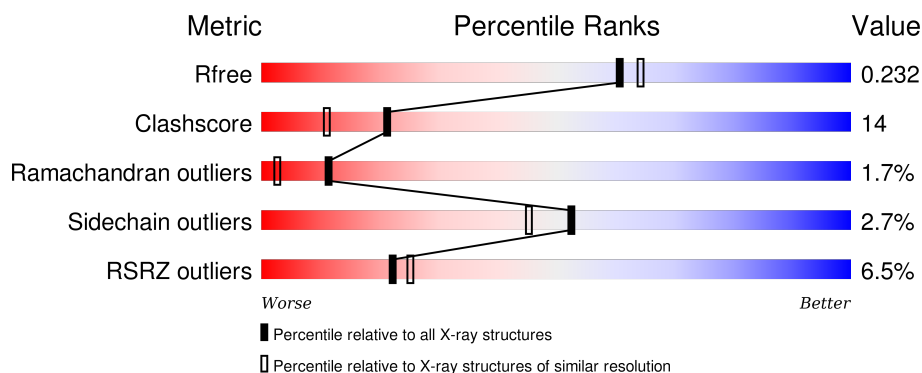
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.03 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	1192 (2.04-2.04)
Clashscore	102246	1269 (2.04-2.04)
Ramachandran outliers	100387	1258 (2.04-2.04)
Sidechain outliers	100360	1258 (2.04-2.04)
RSRZ outliers	91569	1194 (2.04-2.04)

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	258	<div> <div>7%</div> <div> <div></div> <div>72%</div> <div>19%</div> <div>•• 7%</div> </div> </div>
1	B	258	<div> <div>7%</div> <div> <div></div> <div>72%</div> <div>19%</div> <div>•• 7%</div> </div> </div>
2	C	258	<div> <div>5%</div> <div> <div></div> <div>72%</div> <div>17%</div> <div>• 9%</div> </div> </div>
2	D	258	<div> <div>5%</div> <div> <div></div> <div>70%</div> <div>16%</div> <div>• 11%</div> </div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7813 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 Estrogen receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	241	Total	C	N	O	S	0	1	0
			1896	1213	321	342	20			
1	B	241	Total	C	N	O	S	0	1	0
			1891	1210	321	341	19			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	296	SER	-	expression tag	UNP P03372
A	297	ASN	-	expression tag	UNP P03372
A	298	ALA	-	expression tag	UNP P03372
A	372	ARG	LEU	engineered	UNP P03372
A	536	SER	LEU	engineered	UNP P03372
B	296	SER	-	expression tag	UNP P03372
B	297	ASN	-	expression tag	UNP P03372
B	298	ALA	-	expression tag	UNP P03372
B	372	ARG	LEU	engineered	UNP P03372
B	536	SER	LEU	engineered	UNP P03372

- Molecule 2 is a protein called Estrogen receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	234	Total	C	N	O	S	0	2	0
			1841	1177	314	331	19			
2	D	230	Total	C	N	O	S	0	1	0
			1806	1156	307	324	19			

There are 10 discrepancies between the modelled and reference sequences:

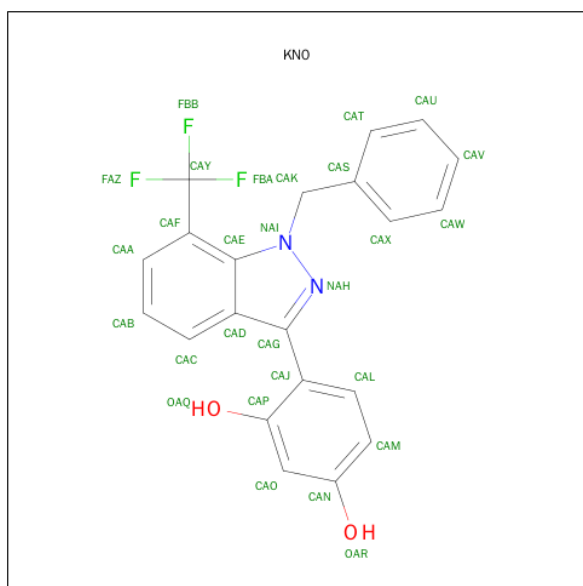
Chain	Residue	Modelled	Actual	Comment	Reference
C	296	SER	-	expression tag	UNP P03372
C	297	ASN	-	expression tag	UNP P03372

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Chain	Residue	Modelled	Actual	Comment	Reference
C	298	ALA	-	expression tag	UNP P03372
C	372	ARG	LEU	engineered	UNP P03372
C	536	SER	LEU	engineered	UNP P03372
D	296	SER	-	expression tag	UNP P03372
D	297	ASN	-	expression tag	UNP P03372
D	298	ALA	-	expression tag	UNP P03372
D	372	ARG	LEU	engineered	UNP P03372
D	536	SER	LEU	engineered	UNP P03372

- Molecule 3 is 4-[1-BENZYL-7-(TRIFLUOROMETHYL)-1H-INDAZOL-3-YL]BENZENE-1,3-DIOL (three-letter code: KNO) (formula: C<sub>21</sub>H<sub>15</sub>F<sub>3</sub>N<sub>2</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 28	C 21	F 3	N 2	O 2	0	0
3	B	1	Total 28	C 21	F 3	N 2	O 2	0	0
3	C	1	Total 28	C 21	F 3	N 2	O 2	0	0
3	D	1	Total 28	C 21	F 3	N 2	O 2	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	60	Total	O	0	0
			60	60		

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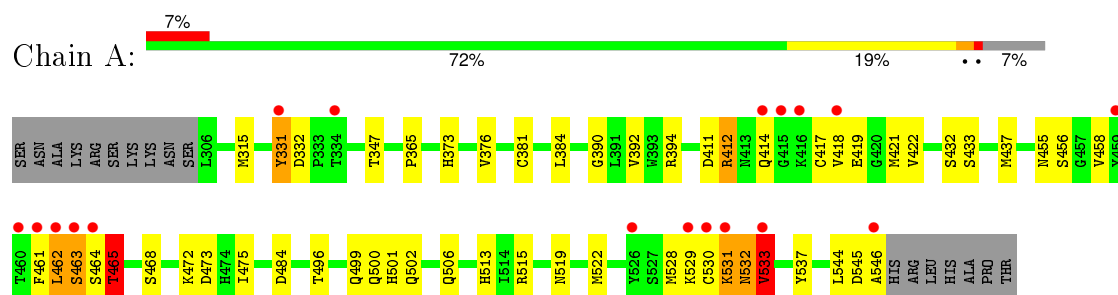
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	76	Total 76	O 76	0	0
4	C	66	Total 66	O 66	0	0
4	D	65	Total 65	O 65	0	0

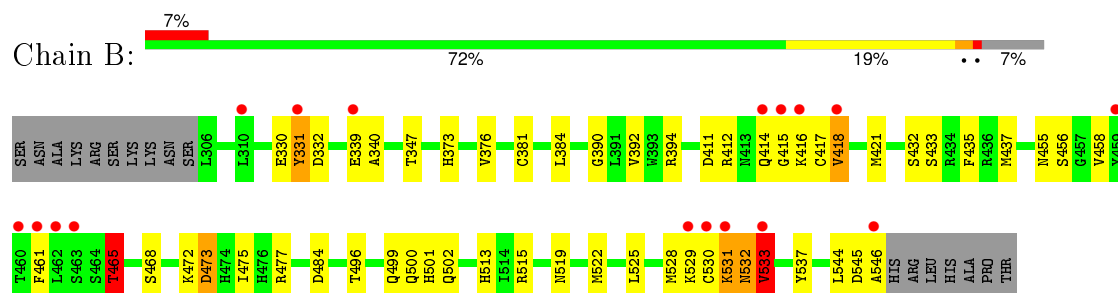
### 3 Residue-property plots [i](#)

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.

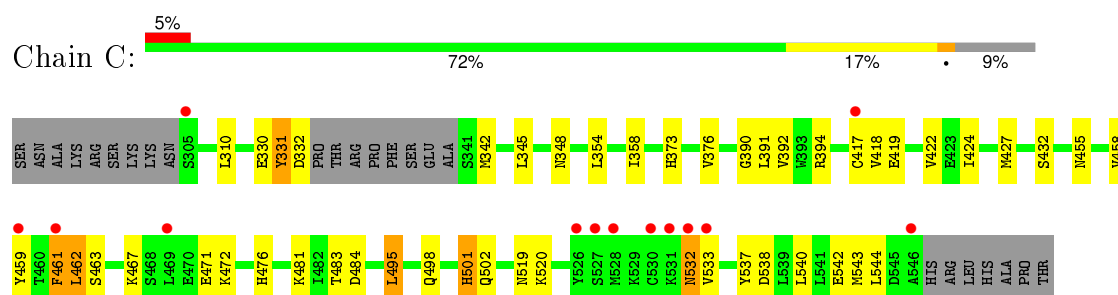
#### • Molecule 1: Estrogen receptor



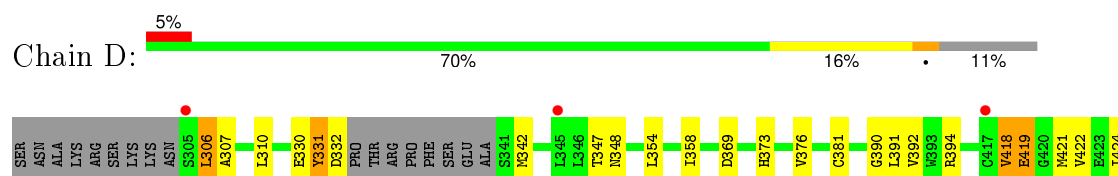
#### • Molecule 1: Estrogen receptor



#### • Molecule 2: Estrogen receptor



#### • Molecule 2: Estrogen receptor





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	53.70Å 58.57Å 93.46Å 80.40° 74.85° 62.79°	Depositor
Resolution (Å)	38.20 – 2.03 45.04 – 2.03	Depositor EDS
% Data completeness (in resolution range)	73.4 (38.20-2.03) 77.7 (45.04-2.03)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.46 (at 2.03Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6 _289)	Depositor
R, $R_{free}$	0.186 , 0.228 0.190 , 0.232	Depositor DCC
$R_{free}$ test set	2499 reflections (5.35%)	DCC
Wilson B-factor (Å <sup>2</sup> )	34.7	Xtriage
Anisotropy	0.428	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 56.4	EDS
Estimated twinning fraction	0.138 for h,h-k,h-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 49194 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	7813	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.14% 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: CME, KN0

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	0.26	0/1925	0.46	0/2606
1	B	0.26	0/1920	0.47	0/2601
2	C	0.26	0/1880	0.42	0/2541
2	D	0.26	0/1840	0.41	0/2486
All	All	0.26	0/7565	0.44	0/10234

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	532	ASN	Peptide
1	B	532	ASN	Peptide

## 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	1896	0	1903	59	0
1	B	1891	0	1890	55	0
2	C	1841	0	1861	55	0
2	D	1806	0	1823	54	0
3	A	28	0	14	2	0
3	B	28	0	13	4	0
3	C	28	0	13	7	0
3	D	28	0	13	8	0
4	A	60	0	0	2	0
4	B	76	0	0	2	0
4	C	66	0	0	0	0
4	D	65	0	0	1	0
All	All	7813	0	7530	214	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 14.

All (214) 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)
2:C:342:MET:HE3	2:C:418:VAL:HG11	1.27	1.07
1:A:331:TYR:HD1	1:A:332:ASP:N	1.56	1.04
1:B:331:TYR:HD1	1:B:332:ASP:N	1.56	1.04
1:A:519:ASN:HD22	2:C:519:ASN:HD22	0.95	0.91
1:B:519:ASN:HD22	2:D:519:ASN:HD22	0.91	0.88
2:C:533:VAL:HG11	3:C:1:KN0:HAV	1.59	0.85
1:A:462:LEU:HA	1:A:463:SER:CB	2.06	0.84
2:D:501[A]:HIS:HD2	2:D:502:GLN:N	1.77	0.82
1:A:331:TYR:CD1	1:A:332:ASP:N	2.47	0.81
1:B:331:TYR:CD1	1:B:332:ASP:N	2.47	0.81
2:C:501[A]:HIS:HD2	2:C:502:GLN:N	1.79	0.79
3:A:1:KN0:HAC	3:A:1:KN0:HAL	1.66	0.78
2:C:501[A]:HIS:CD2	2:C:502:GLN:HG3	2.19	0.77
2:D:501[A]:HIS:CD2	2:D:502:GLN:N	2.53	0.77
2:D:501[A]:HIS:CD2	2:D:502:GLN:HG3	2.20	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:373:HIS:HD2	1:A:537:TYR:OH	1.70	0.75
2:C:342:MET:CE	2:C:418:VAL:HG11	2.14	0.75
2:C:501[A]:HIS:CD2	2:C:502:GLN:N	2.55	0.75
1:B:519:ASN:HD22	2:D:519:ASN:ND2	1.77	0.74
1:B:373:HIS:HD2	1:B:537:TYR:OH	1.70	0.74
2:C:458:VAL:HG13	2:C:459:TYR:CD1	2.23	0.73
1:A:419:GLU:HA	1:A:422:VAL:HG13	1.69	0.72
2:C:310:LEU:O	2:C:481:LYS:HE2	1.88	0.72
2:D:310:LEU:O	2:D:481:LYS:HE2	1.88	0.72
2:C:533:VAL:HG11	3:C:1:KN0:CAV	2.19	0.72
1:B:519:ASN:ND2	2:D:519:ASN:HD22	1.77	0.71
2:D:458:VAL:HG13	2:D:459:TYR:CD1	2.24	0.71
2:D:533:VAL:HG11	3:D:1:KN0:CAV	2.20	0.71
2:D:533:VAL:HG11	3:D:1:KN0:HAV	1.72	0.69
1:A:456:SER:HA	1:A:515:ARG:NH2	2.08	0.69
1:B:456:SER:HA	1:B:515:ARG:NH2	2.08	0.69
1:A:519:ASN:ND2	2:C:519:ASN:HD22	1.80	0.68
1:B:339:GLU:HA	1:B:416:LYS:O	1.94	0.68
3:D:1:KN0:HAC	3:D:1:KN0:HAL	1.75	0.68
3:B:1:KN0:HAL	3:B:1:KN0:HAC	1.76	0.67
1:A:381:CYS:SG	4:A:135:HOH:O	2.52	0.66
1:A:331:TYR:HD1	1:A:332:ASP:H	1.42	0.65
1:B:331:TYR:HD1	1:B:332:ASP:H	1.43	0.64
2:D:306:LEU:HD23	2:D:306:LEU:N	2.13	0.64
2:C:461:PHE:O	2:C:462:LEU:CB	2.46	0.64
3:D:1:KN0:HAK	3:D:1:KN0:FBB	1.88	0.63
1:A:506:GLN:NE2	2:C:476[B]:HIS:HE1	1.97	0.63
1:A:461:PHE:HE2	1:A:475:ILE:HD12	1.63	0.63
1:A:417:CME:HB2	1:A:421:MET:HB2	1.81	0.62
3:C:1:KN0:HAC	3:C:1:KN0:HAL	1.83	0.61
1:A:501[B]:HIS:CD2	1:A:502:GLN:HG3	2.36	0.61
2:D:532:ASN:ND2	2:D:532:ASN:H	1.99	0.61
1:B:461:PHE:HE2	1:B:475:ILE:HD12	1.66	0.60
2:C:532:ASN:H	2:C:532:ASN:ND2	1.99	0.60
1:B:501[B]:HIS:CD2	1:B:502:GLN:HG3	2.36	0.60
2:D:342:MET:HG2	2:D:418:VAL:HG11	1.83	0.59
1:A:392:VAL:HG13	1:A:432:SER:HA	1.82	0.59
2:C:501[A]:HIS:NE2	2:C:502:GLN:HG3	2.17	0.59
2:D:532:ASN:N	2:D:532:ASN:HD22	2.00	0.59
1:A:461:PHE:HD2	1:A:472:LYS:HG2	1.66	0.59
2:C:532:ASN:HD22	2:C:532:ASN:N	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:458:VAL:HG13	2:C:459:TYR:HD1	1.67	0.59
1:B:392:VAL:HG13	1:B:432:SER:HA	1.82	0.59
2:D:501[A]:HIS:NE2	2:D:502:GLN:HG3	2.18	0.59
1:A:461:PHE:CD2	1:A:472:LYS:HG2	2.37	0.59
1:B:461:PHE:HD2	1:B:472:LYS:HG2	1.66	0.59
1:B:461:PHE:CD2	1:B:472:LYS:HG2	2.38	0.58
1:B:331:TYR:CD1	1:B:332:ASP:HB2	2.38	0.58
1:B:501[B]:HIS:CD2	1:B:502:GLN:N	2.71	0.58
2:D:458:VAL:HG13	2:D:459:TYR:HD1	1.68	0.58
1:A:501[B]:HIS:CD2	1:A:502:GLN:N	2.71	0.58
1:A:331:TYR:CD1	1:A:332:ASP:HB2	2.39	0.58
1:B:513:HIS:HE1	2:D:455:ASN:O	1.88	0.57
1:B:496:THR:O	1:B:500:GLN:HG3	2.05	0.57
1:B:415:GLY:O	1:B:417:CME:HE2	2.04	0.57
1:A:484:ASP:OD1	2:C:501[A]:HIS:NE2	2.38	0.56
1:A:347:THR:HG23	1:A:533:VAL:HB	1.87	0.56
1:A:496:THR:O	1:A:500:GLN:HG3	2.06	0.56
2:D:532:ASN:N	2:D:532:ASN:ND2	2.54	0.56
2:C:376:VAL:HG22	2:C:544:LEU:HD12	1.87	0.56
2:C:532:ASN:ND2	2:C:532:ASN:N	2.54	0.56
1:B:525:LEU:HD21	3:B:1:KN0:HAA	1.88	0.56
1:B:465:THR:HG23	1:B:468:SER:HB2	1.88	0.56
1:B:347:THR:HG23	1:B:533:VAL:HB	1.88	0.56
1:A:531:LYS:CB	2:D:422:VAL:HG21	2.36	0.55
1:A:465:THR:HG23	1:A:468:SER:HB2	1.89	0.55
2:D:306:LEU:HD21	2:D:369:ASP:OD2	2.06	0.55
2:C:373:HIS:HD2	2:C:537:TYR:OH	1.89	0.55
1:B:531:LYS:CB	2:C:422:VAL:HG21	2.36	0.55
2:C:391:LEU:HB2	3:C:1:KN0:HAM	1.89	0.55
2:D:538:ASP:O	2:D:542:GLU:HG2	2.07	0.54
2:D:306:LEU:CD2	2:D:306:LEU:N	2.70	0.54
2:D:306:LEU:H	2:D:306:LEU:HD23	1.71	0.54
2:D:373:HIS:HD2	2:D:537:TYR:OH	1.91	0.54
2:C:424:ILE:HA	2:C:427:MET:HE2	1.90	0.53
2:C:538:ASP:O	2:C:542:GLU:HG2	2.08	0.53
2:D:376:VAL:HG22	2:D:544:LEU:HD12	1.90	0.53
2:D:461:PHE:HB2	2:D:472:LYS:HE3	1.91	0.52
3:C:1:KN0:CAY	3:C:1:KN0:HAK	2.39	0.52
2:D:424:ILE:HA	2:D:427:MET:HE2	1.91	0.52
1:A:461:PHE:CE2	1:A:475:ILE:HD12	2.44	0.52
1:B:513:HIS:CE1	2:D:455:ASN:O	2.63	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:473:ASP:HB3	1:B:477:ARG:HH21	1.74	0.52
1:B:381:CYS:SG	4:B:130:HOH:O	2.46	0.52
3:B:1:KN0:FBB	3:B:1:KN0:HAKA	2.00	0.51
1:A:519:ASN:HD22	2:C:519:ASN:ND2	1.81	0.51
3:A:1:KN0:HAL	3:A:1:KN0:CAC	2.36	0.51
1:B:330:GLU:HG3	4:B:71:HOH:O	2.10	0.51
3:D:1:KN0:HAL	3:D:1:KN0:CAC	2.41	0.51
1:A:433:SER:O	1:A:437:MET:HG2	2.11	0.51
1:A:545:ASP:O	1:A:546:ALA:C	2.49	0.51
2:C:461:PHE:HB2	2:C:472:LYS:HE3	1.93	0.50
1:B:411:ASP:OD1	1:B:414:GLN:HG3	2.10	0.50
2:D:354:LEU:O	2:D:358:ILE:HD13	2.11	0.50
2:C:330:GLU:O	2:C:331:TYR:CB	2.58	0.50
2:C:373:HIS:CD2	2:C:537:TYR:OH	2.63	0.50
2:D:330:GLU:O	2:D:331:TYR:CB	2.59	0.50
2:D:424:ILE:HA	2:D:427:MET:CE	2.42	0.50
1:A:455:ASN:O	1:A:458:VAL:HG12	2.12	0.50
2:D:373:HIS:CD2	2:D:537:TYR:OH	2.65	0.49
2:C:424:ILE:HA	2:C:427:MET:CE	2.42	0.49
1:B:331:TYR:CE1	1:B:332:ASP:HB2	2.47	0.49
1:A:411:ASP:OD1	1:A:414:GLN:HG3	2.11	0.49
2:D:306:LEU:HD23	2:D:307:ALA:H	1.77	0.49
1:B:461:PHE:CE2	1:B:475:ILE:HD12	2.46	0.49
1:B:433:SER:O	1:B:437:MET:HG2	2.12	0.49
1:A:373:HIS:CD2	1:A:537:TYR:OH	2.59	0.49
2:D:467:LYS:O	2:D:471:GLU:HG2	2.12	0.49
1:A:331:TYR:CE1	1:A:332:ASP:HB2	2.48	0.49
2:C:498:GLN:O	2:C:501[A]:HIS:CD2	2.66	0.49
1:B:373:HIS:CD2	1:B:537:TYR:OH	2.60	0.48
2:D:498:GLN:O	2:D:501[A]:HIS:CD2	2.67	0.48
1:B:545:ASP:O	1:B:546:ALA:C	2.51	0.48
2:C:467:LYS:O	2:C:471:GLU:HG2	2.13	0.48
2:D:391:LEU:HB2	3:D:1:KN0:HAM	1.96	0.48
2:C:390:GLY:O	2:C:394:ARG:HG3	2.13	0.48
1:B:455:ASN:O	1:B:458:VAL:HG12	2.13	0.48
1:A:513:HIS:NE2	2:C:459:TYR:CE1	2.82	0.48
2:C:342:MET:HE3	2:C:418:VAL:CG1	2.19	0.47
1:A:513:HIS:HE1	2:C:455:ASN:O	1.98	0.47
3:D:1:KN0:CAY	3:D:1:KN0:HAK	2.44	0.47
2:C:354:LEU:O	2:C:358:ILE:HD13	2.14	0.47
1:B:501[B]:HIS:CD2	2:D:483:THR:HG22	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:1:KN0:HAL	3:B:1:KN0:CAC	2.44	0.47
1:B:376:VAL:HG22	1:B:544:LEU:HD12	1.96	0.47
2:C:330:GLU:HG2	2:C:348:ASN:OD1	2.15	0.46
2:D:347:THR:HA	3:D:1:KN0:HAV	1.98	0.46
1:A:376:VAL:HG22	1:A:544:LEU:HD12	1.96	0.46
2:C:418:VAL:HG23	2:C:418:VAL:O	2.16	0.46
1:A:392:VAL:HG13	1:A:432:SER:CA	2.45	0.46
2:D:330:GLU:HG2	2:D:348:ASN:OD1	2.16	0.46
2:D:392:VAL:HG13	2:D:432:SER:HA	1.98	0.45
1:A:496:THR:OG1	1:A:499:GLN:HG3	2.17	0.45
1:A:390:GLY:O	1:A:394:ARG:HG3	2.17	0.45
2:D:390:GLY:O	2:D:394:ARG:HG3	2.16	0.45
3:C:1:KN0:FBB	3:C:1:KN0:HAK	2.06	0.45
1:A:384:LEU:HD23	1:A:522:MET:HE2	1.98	0.45
1:B:331:TYR:C	1:B:331:TYR:CD1	2.84	0.45
1:A:331:TYR:CD1	1:A:331:TYR:C	2.85	0.45
1:A:501[B]:HIS:NE2	1:A:502:GLN:HG3	2.32	0.45
1:A:531:LYS:O	1:A:532:ASN:HB2	2.16	0.44
1:B:465:THR:HG23	1:B:468:SER:CB	2.46	0.44
2:C:501[A]:HIS:HE2	2:C:502:GLN:HG3	1.81	0.44
1:B:501[B]:HIS:NE2	1:B:502:GLN:HG3	2.33	0.44
2:D:501[A]:HIS:HE2	2:D:502:GLN:HG3	1.82	0.44
2:D:418:VAL:O	2:D:419:GLU:C	2.56	0.44
1:A:501[B]:HIS:NE2	2:C:484:ASP:OD1	2.47	0.44
2:D:381:CYS:SG	4:D:134:HOH:O	2.48	0.44
1:B:484:ASP:OD1	2:D:501[A]:HIS:NE2	2.49	0.44
1:B:513:HIS:NE2	2:D:459:TYR:CE1	2.86	0.44
2:C:463:SER:H	2:C:472:LYS:HZ1	1.65	0.44
1:B:532:ASN:O	1:B:533:VAL:HG12	2.16	0.44
1:A:530:CYS:O	1:A:532:ASN:N	2.51	0.43
1:A:532:ASN:O	1:A:533:VAL:HG12	2.16	0.43
3:C:1:KN0:CAC	3:C:1:KN0:HAL	2.48	0.43
1:A:384:LEU:CD2	1:A:522:MET:HE2	2.48	0.43
1:B:390:GLY:O	1:B:394:ARG:HG3	2.19	0.43
1:A:513:HIS:CE1	2:C:459:TYR:CD1	3.06	0.43
2:D:418:VAL:HB	2:D:421:MET:HB2	2.01	0.43
1:B:392:VAL:HG13	1:B:432:SER:CA	2.48	0.43
1:A:465:THR:HG23	1:A:468:SER:CB	2.48	0.43
2:D:542:GLU:HG2	2:D:542:GLU:H	1.68	0.43
1:A:513:HIS:CE1	2:C:455:ASN:O	2.72	0.42
2:C:542:GLU:HG2	2:C:542:GLU:H	1.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:392:VAL:HG13	2:C:432:SER:HA	2.00	0.42
1:B:339:GLU:HG3	1:B:340:ALA:N	2.35	0.42
1:B:418:VAL:O	1:B:421:MET:HB2	2.19	0.42
1:A:418:VAL:O	1:A:421:MET:HB2	2.20	0.42
1:A:412:ARG:HB3	4:A:36:HOH:O	2.19	0.42
1:A:315:MET:SD	1:A:365:PRO:HG2	2.59	0.42
1:B:384:LEU:CD2	1:B:522:MET:HE2	2.50	0.42
1:B:384:LEU:HD23	1:B:522:MET:HE2	2.00	0.42
1:B:530:CYS:O	1:B:532:ASN:N	2.53	0.42
1:B:392:VAL:HG12	1:B:435:PHE:HD2	1.85	0.41
2:C:331:TYR:O	2:C:332:ASP:C	2.57	0.41
2:C:495:LEU:HD23	2:C:495:LEU:N	2.35	0.41
1:A:501[B]:HIS:CD2	2:C:483:THR:HG22	2.55	0.41
2:D:540:LEU:HA	2:D:543:MET:HE2	2.02	0.41
1:A:528:MET:C	1:A:530:CYS:H	2.23	0.41
1:B:496:THR:OG1	1:B:499:GLN:HG3	2.20	0.41
2:D:331:TYR:O	2:D:332:ASP:C	2.58	0.41
2:C:501[A]:HIS:HD2	2:C:502:GLN:CA	2.33	0.41
2:C:520:LYS:HA	2:C:520:LYS:HD2	1.84	0.41
2:C:345:LEU:HD23	2:C:345:LEU:HA	1.89	0.41
1:B:528:MET:C	1:B:530:CYS:H	2.23	0.41
1:A:513:HIS:NE2	2:C:459:TYR:CD1	2.89	0.41
2:C:540:LEU:HA	2:C:543:MET:HE2	2.02	0.41
2:D:495:LEU:N	2:D:495:LEU:HD23	2.36	0.41
1:B:501[B]:HIS:HD2	1:B:502:GLN:N	2.16	0.41
2:D:540:LEU:HD23	2:D:543:MET:HE3	2.02	0.41
1:A:501[B]:HIS:HD2	1:A:502:GLN:N	2.16	0.41
1:A:530:CYS:C	1:A:532:ASN:H	2.24	0.41
1:B:411:ASP:CG	1:B:414:GLN:HG3	2.41	0.40
2:D:520:LYS:HA	2:D:520:LYS:HD2	1.84	0.40
1:A:464:SER:O	1:A:465:THR:O	2.40	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	239/258 (93%)	228 (95%)	5 (2%)	6 (2%)	7	1
1	B	239/258 (93%)	228 (95%)	7 (3%)	4 (2%)	11	3
2	C	232/258 (90%)	226 (97%)	3 (1%)	3 (1%)	15	5
2	D	225/258 (87%)	219 (97%)	3 (1%)	3 (1%)	15	5
All	All	935/1032 (91%)	901 (96%)	18 (2%)	16 (2%)	11	3

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	462	LEU
1	A	463	SER
1	A	465	THR
1	B	465	THR
2	C	331	TYR
2	C	419	GLU
2	C	462	LEU
2	D	331	TYR
2	D	419	GLU
2	D	546	ALA
1	A	531	LYS
1	B	531	LYS
1	A	529	LYS
1	B	529	LYS
1	B	533	VAL
1	A	533	VAL

### 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	207/231 (90%)	202 (98%)	5 (2%)	57	50
1	B	205/231 (89%)	199 (97%)	6 (3%)	50	42

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	C	204/232 (88%)	198 (97%)	6 (3%)	50	42
2	D	199/232 (86%)	192 (96%)	7 (4%)	43	35
All	All	815/926 (88%)	791 (97%)	24 (3%)	52	42

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	331	TYR
1	A	412	ARG
1	A	465	THR
1	A	473	ASP
1	A	533	VAL
1	B	331	TYR
1	B	412	ARG
1	B	418	VAL
1	B	465	THR
1	B	473	ASP
1	B	533	VAL
2	C	417	CYS
2	C	461	PHE
2	C	495	LEU
2	C	501[A]	HIS
2	C	501[B]	HIS
2	C	532	ASN
2	D	306	LEU
2	D	418	VAL
2	D	461	PHE
2	D	495	LEU
2	D	501[A]	HIS
2	D	501[B]	HIS
2	D	532	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	373	HIS
1	A	519	ASN
1	B	373	HIS
1	B	519	ASN
2	C	373	HIS

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Mol	Chain	Res	Type
2	C	455	ASN
2	C	488	HIS
2	C	502	GLN
2	C	513	HIS
2	C	532	ASN
2	D	356	HIS
2	D	373	HIS
2	D	455	ASN
2	D	502	GLN
2	D	513	HIS
2	D	532	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 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	CME	A	417	1	8,9,10	0.82	0	6,9,11	1.36	0
1	CME	B	417	1	8,9,10	0.77	0	6,9,11	1.62	1 (16%)

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	CME	A	417	1	-	0/5/8/10	0/0/0/0
1	CME	B	417	1	-	0/5/8/10	0/0/0/0

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	B	417	CME	CB-SG-SD	2.70	109.21	103.95

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	417	CME	1	0
1	B	417	CME	1	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
3	KN0	A	1	-	28,31,31	2.06	3 (10%)	36,46,46	1.73	4 (11%)
3	KN0	B	1	-	28,31,31	2.17	3 (10%)	36,46,46	1.63	5 (13%)
3	KN0	C	1	-	28,31,31	2.11	4 (14%)	36,46,46	1.40	4 (11%)
3	KN0	D	1	-	28,31,31	2.04	4 (14%)	36,46,46	1.59	4 (11%)

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	KN0	A	1	-	-	0/12/14/14	0/4/4/4
3	KN0	B	1	-	-	0/12/14/14	0/4/4/4
3	KN0	C	1	-	-	0/12/14/14	0/4/4/4
3	KN0	D	1	-	-	0/12/14/14	0/4/4/4

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1	KN0	CAJ-CAG	-9.99	1.39	1.49
3	A	1	KN0	CAJ-CAG	-9.31	1.40	1.49
3	C	1	KN0	CAJ-CAG	-9.20	1.40	1.49
3	D	1	KN0	CAJ-CAG	-9.02	1.40	1.49
3	C	1	KN0	CAF-CAE	-2.74	1.39	1.42
3	C	1	KN0	CAG-NAH	-2.59	1.32	1.35
3	B	1	KN0	CAF-CAE	-2.47	1.40	1.42
3	D	1	KN0	CAF-CAE	-2.41	1.40	1.42
3	A	1	KN0	CAF-CAE	-2.21	1.40	1.42
3	D	1	KN0	CAG-NAH	-2.08	1.33	1.35
3	B	1	KN0	CAY-CAF	3.24	1.54	1.50
3	A	1	KN0	CAY-CAF	3.41	1.54	1.50
3	D	1	KN0	CAY-CAF	3.77	1.55	1.50
3	C	1	KN0	CAY-CAF	3.85	1.55	1.50

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1	KN0	FBB-CAY-CAF	-5.38	107.15	112.39
3	B	1	KN0	FBB-CAY-CAF	-4.71	107.81	112.39
3	D	1	KN0	FAZ-CAY-CAF	-3.94	108.56	112.39
3	C	1	KN0	FAZ-CAY-CAF	-3.82	108.68	112.39
3	B	1	KN0	CAP-CAJ-CAG	-2.86	118.19	121.48
3	B	1	KN0	FAZ-CAY-CAF	-2.77	109.69	112.39
3	D	1	KN0	FBA-CAY-CAF	-2.60	109.86	112.39
3	A	1	KN0	FAZ-CAY-CAF	-2.29	110.16	112.39
3	C	1	KN0	CAP-CAJ-CAG	-2.18	118.96	121.48
3	C	1	KN0	CAY-CAF-CAE	3.22	121.61	119.58
3	C	1	KN0	CAJ-CAG-NAH	4.18	126.10	120.71
3	B	1	KN0	CAY-CAF-CAE	4.32	122.30	119.58
3	D	1	KN0	CAY-CAF-CAE	4.70	122.53	119.58
3	B	1	KN0	CAJ-CAG-NAH	4.78	126.88	120.71
3	A	1	KN0	CAY-CAF-CAE	4.98	122.71	119.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1	KN0	CAJ-CAG-NAH	5.21	127.44	120.71
3	D	1	KN0	CAJ-CAG-NAH	5.24	127.47	120.71

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1	KN0	2	0
3	B	1	KN0	4	0
3	C	1	KN0	7	0
3	D	1	KN0	8	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<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	240/258 (93%)	0.24	18 (7%)	17 20	25, 42, 107, 131	2 (0%)
1	B	240/258 (93%)	0.26	17 (7%)	19 22	25, 41, 100, 130	2 (0%)
2	C	234/258 (90%)	0.19	13 (5%)	28 32	26, 41, 93, 111	2 (0%)
2	D	230/258 (89%)	0.19	13 (5%)	27 31	26, 40, 97, 128	2 (0%)
All	All	944/1032 (91%)	0.22	61 (6%)	22 25	25, 41, 99, 131	8 (0%)

All (61) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	459	TYR	5.6
1	B	462	LEU	5.3
1	A	416	LYS	5.1
1	B	533	VAL	4.8
2	D	417	CYS	4.8
1	A	415	GLY	4.7
1	B	530	CYS	4.6
1	B	463	SER	4.4
2	C	459	TYR	4.3
1	A	533	VAL	4.0
2	D	460	THR	3.9
2	C	532	ASN	3.8
1	A	546	ALA	3.7
1	A	331	TYR	3.7
1	A	418	VAL	3.7
1	B	331	TYR	3.7
1	B	461	PHE	3.6
2	C	530	CYS	3.6
2	D	531	LYS	3.5
1	B	339	GLU	3.5
2	C	528	MET	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	461	PHE	3.4
2	D	528	MET	3.4
1	B	529	LYS	3.3
2	C	546	ALA	3.3
1	B	460	THR	3.2
2	D	533	VAL	3.2
1	A	459	TYR	3.2
1	B	415	GLY	3.1
2	D	305	SER	3.1
1	A	526	TYR	2.9
1	B	531	LYS	2.9
2	C	533	VAL	2.9
2	D	545	ASP	2.8
2	D	529	LYS	2.8
2	D	532	ASN	2.8
2	D	547	HIS	2.7
1	A	463	SER	2.7
2	D	546	ALA	2.7
2	C	526	TYR	2.7
1	A	530	CYS	2.6
1	A	462	LEU	2.6
1	A	414	GLN	2.6
1	A	334	THR	2.6
2	C	417	CYS	2.5
2	D	345	LEU	2.5
1	B	416	LYS	2.5
2	C	461	PHE	2.4
1	B	546	ALA	2.3
1	B	418	VAL	2.3
1	A	529	LYS	2.3
1	B	414	GLN	2.2
1	B	459	TYR	2.2
1	A	464	SER	2.2
2	C	305	SER	2.2
2	C	527	SER	2.1
1	A	531	LYS	2.1
2	C	531	LYS	2.1
1	B	310	LEU	2.1
2	C	469	LEU	2.1
1	A	460	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	CME	A	417	10/11	0.88	0.26	-	67,100,104,105	0
1	CME	B	417	10/11	0.78	0.26	-	66,85,90,136	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(Å <sup>2</sup> )	Q<0.9
3	KN0	C	1	28/28	0.90	0.16	0.78	39,50,64,68	0
3	KN0	D	1	28/28	0.90	0.14	0.34	36,46,59,65	0
3	KN0	B	1	28/28	0.93	0.13	0.03	29,39,50,51	0
3	KN0	A	1	28/28	0.95	0.11	-0.16	23,42,50,52	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.