Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 03:30 PM GMT

PDB ID	:	4CCK
Title	:	60S ribosomal protein L8 histidine hydroxylase (NO66) in complex with Mn(II) and N-oxalylglycine (NOG)
Authors	:	Chowdhury, R.; Ge, W.; Clifton, I.J.; Schofield, C.J.
Deposited on	:	2013-10-23
Resolution	:	2.15 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

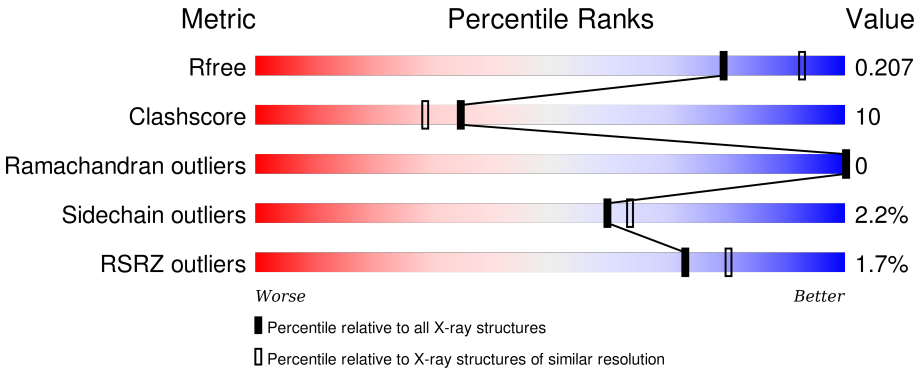
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.15 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	1045 (2.16-2.16)
Clashscore	102246	1152 (2.16-2.16)
Ramachandran outliers	100387	1131 (2.16-2.16)
Sidechain outliers	100360	1131 (2.16-2.16)
RSRZ outliers	91569	1050 (2.16-2.16)

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	467	79% 18%
1	B	467	3% 77% 19%
1	C	467	2% 82% 15%
1	D	467	% 72% 25%

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
4	EDO	B	903	-	-	-	X
4	EDO	C	903	-	-	-	X
4	EDO	D	903	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 15509 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 BIFUNCTIONAL LYSINE-SPECIFIC DEMETHYLASE AND HISTIDYL-HYDROXYLASE NO66.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	456	Total	C	N	O	S	0	2	0
			3662	2330	648	668	16			
1	B	456	Total	C	N	O	S	0	4	0
			3641	2329	637	659	16			
1	C	458	Total	C	N	O	S	0	4	0
			3663	2336	641	670	16			
1	D	459	Total	C	N	O	S	0	3	0
			3654	2331	639	668	16			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	182	MET	-	EXPRESSION TAG	UNP Q9H6W3
A	642	ALA	-	EXPRESSION TAG	UNP Q9H6W3
A	643	GLU	-	EXPRESSION TAG	UNP Q9H6W3
A	644	ASN	-	EXPRESSION TAG	UNP Q9H6W3
A	645	LEU	-	EXPRESSION TAG	UNP Q9H6W3
A	646	TYR	-	EXPRESSION TAG	UNP Q9H6W3
A	647	PHE	-	EXPRESSION TAG	UNP Q9H6W3
A	648	GLN	-	EXPRESSION TAG	UNP Q9H6W3
A	364	ALA	VAL	ENGINEERED MUTATION	UNP Q9H6W3
B	182	MET	-	EXPRESSION TAG	UNP Q9H6W3
B	642	ALA	-	EXPRESSION TAG	UNP Q9H6W3
B	643	GLU	-	EXPRESSION TAG	UNP Q9H6W3
B	644	ASN	-	EXPRESSION TAG	UNP Q9H6W3
B	645	LEU	-	EXPRESSION TAG	UNP Q9H6W3
B	646	TYR	-	EXPRESSION TAG	UNP Q9H6W3
B	647	PHE	-	EXPRESSION TAG	UNP Q9H6W3
B	648	GLN	-	EXPRESSION TAG	UNP Q9H6W3
B	364	ALA	VAL	ENGINEERED MUTATION	UNP Q9H6W3
C	182	MET	-	EXPRESSION TAG	UNP Q9H6W3
C	642	ALA	-	EXPRESSION TAG	UNP Q9H6W3

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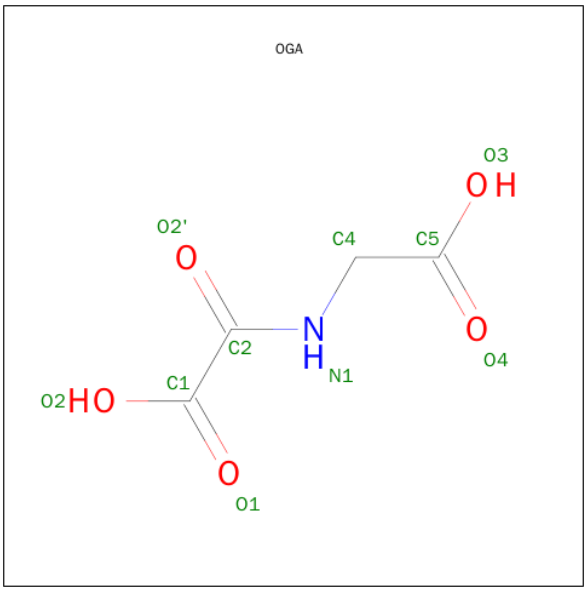
Chain	Residue	Modelled	Actual	Comment	Reference
C	643	GLU	-	EXPRESSION TAG	UNP Q9H6W3
C	644	ASN	-	EXPRESSION TAG	UNP Q9H6W3
C	645	LEU	-	EXPRESSION TAG	UNP Q9H6W3
C	646	TYR	-	EXPRESSION TAG	UNP Q9H6W3
C	647	PHE	-	EXPRESSION TAG	UNP Q9H6W3
C	648	GLN	-	EXPRESSION TAG	UNP Q9H6W3
C	364	ALA	VAL	ENGINEERED MUTATION	UNP Q9H6W3
D	182	MET	-	EXPRESSION TAG	UNP Q9H6W3
D	642	ALA	-	EXPRESSION TAG	UNP Q9H6W3
D	643	GLU	-	EXPRESSION TAG	UNP Q9H6W3
D	644	ASN	-	EXPRESSION TAG	UNP Q9H6W3
D	645	LEU	-	EXPRESSION TAG	UNP Q9H6W3
D	646	TYR	-	EXPRESSION TAG	UNP Q9H6W3
D	647	PHE	-	EXPRESSION TAG	UNP Q9H6W3
D	648	GLN	-	EXPRESSION TAG	UNP Q9H6W3
D	364	ALA	VAL	ENGINEERED MUTATION	UNP Q9H6W3

- Molecule 2 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

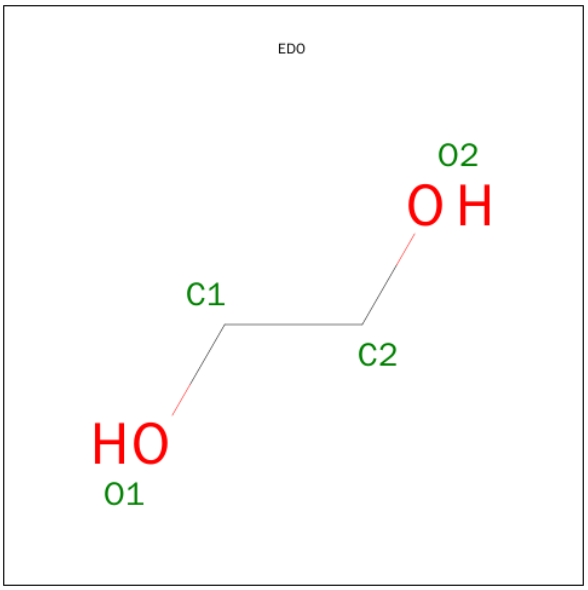
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total Mn 1 1	0	0
2	A	1	Total Mn 1 1	0	0
2	D	1	Total Mn 1 1	0	0
2	C	1	Total Mn 1 1	0	0

- Molecule 3 is N-OXALYLGLYCINE (three-letter code: OGA) (formula: $C_4H_5NO_5$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			10	4	1	5		
3	B	1	Total	C	N	O	0	0
			10	4	1	5		
3	C	1	Total	C	N	O	0	0
			10	4	1	5		
3	D	1	Total	C	N	O	0	0
			10	4	1	5		

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

- Molecule 5 is water.

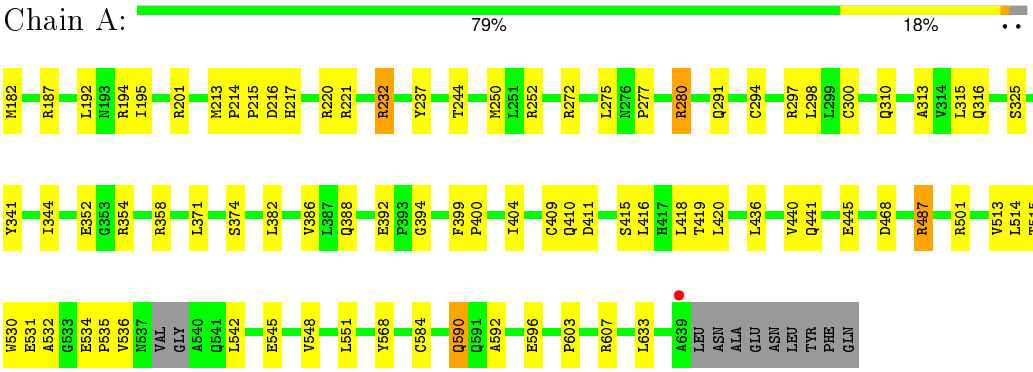
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	278	Total O 278 278	0	0
5	B	170	Total O 170 170	0	0
5	C	236	Total O 236 236	0	0
5	D	145	Total O 145 145	0	0

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.

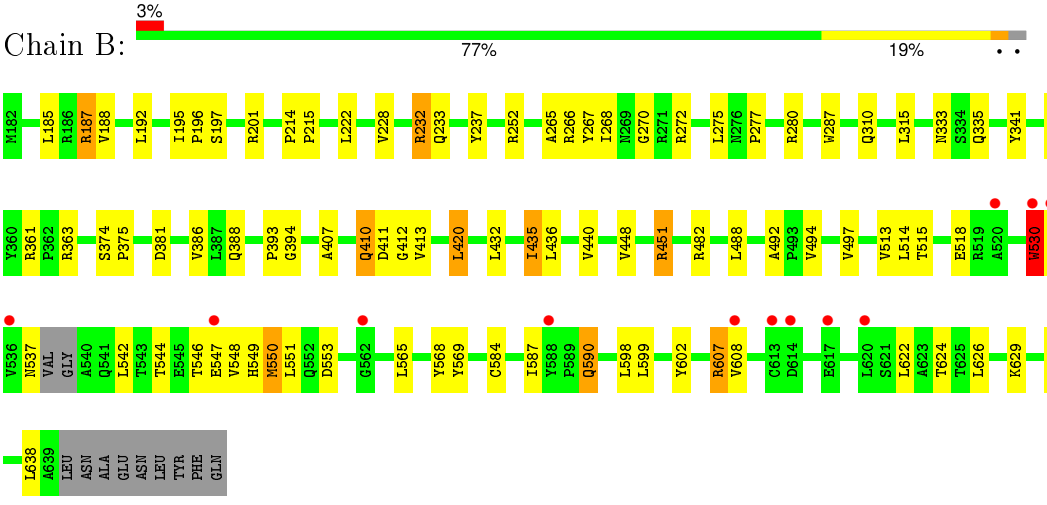
• Molecule 1: BIFUNCTIONAL LYSINE-SPECIFIC DEMETHYLASE AND HISTIDYL-HYDROXYLASE NO66

Chain A:



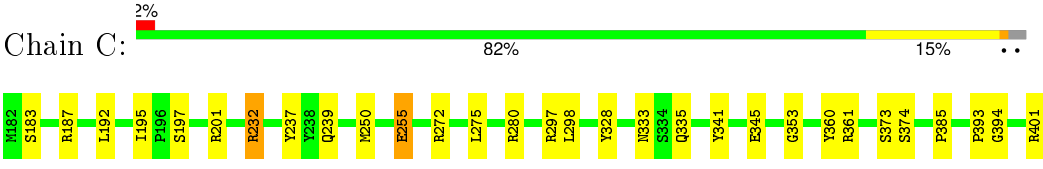
• Molecule 1: BIFUNCTIONAL LYSINE-SPECIFIC DEMETHYLASE AND HISTIDYL-HYDROXYLASE NO66

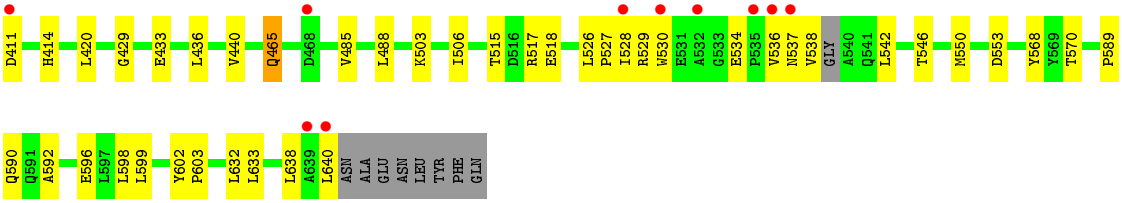
Chain B:



• Molecule 1: BIFUNCTIONAL LYSINE-SPECIFIC DEMETHYLASE AND HISTIDYL-HYDROXYLASE NO66

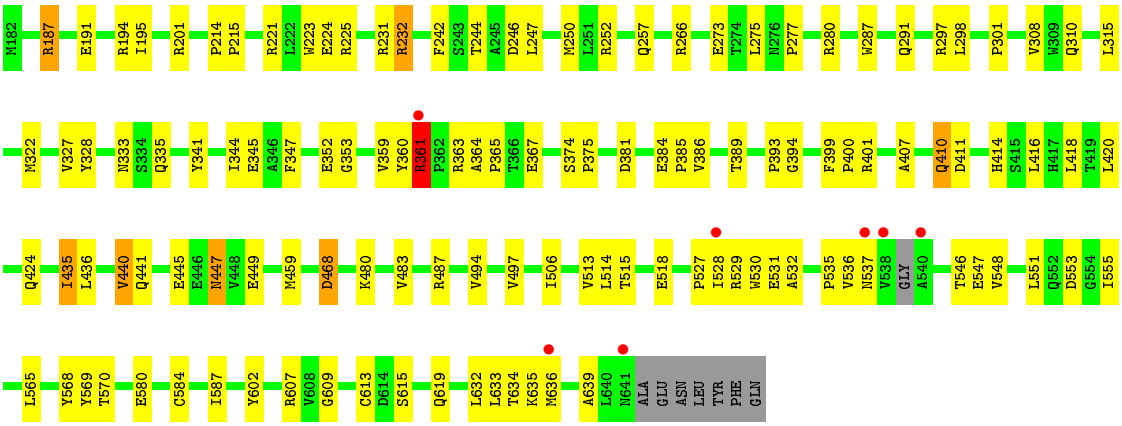
Chain C:





• Molecule 1: BIFUNCTIONAL LYSINE-SPECIFIC DEMETHYLASE AND HISTIDYL-HYDROXYLASE NO66

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	101.41Å 80.71Å 151.54Å 90.00° 94.54° 90.00°	Depositor
Resolution (Å)	81.10 – 2.15 81.10 – 2.15	Depositor EDS
% Data completeness (in resolution range)	98.9 (81.10-2.15) 98.8 (81.10-2.15)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.38 (at 2.16Å)	Xtriage
Refinement program	CNS 1.3	Depositor
R, R_{free}	0.186 , 0.197 0.199 , 0.207	Depositor DCC
R_{free} test set	6595 reflections (5.03%)	DCC
Wilson B-factor (Å^2)	37.9	Xtriage
Anisotropy	0.279	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 43.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Outliers	0 of 131064 reflections	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	15509	wwPDB-VP
Average B, all atoms (Å^2)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.82% 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: MN, OGA, EDO

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	0.35	0/3762	0.62	1/5117 (0.0%)
1	B	0.38	0/3749	0.59	1/5106 (0.0%)
1	C	0.35	0/3769	0.61	1/5131 (0.0%)
1	D	0.32	0/3757	0.58	2/5116 (0.0%)
All	All	0.35	0/15037	0.60	5/20470 (0.0%)

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	2
1	B	0	2
1	C	0	1
1	D	0	4
All	All	0	9

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	361[A]	ARG	CB-CA-C	-5.92	98.57	110.40
1	D	361[B]	ARG	CB-CA-C	-5.92	98.57	110.40
1	A	548	VAL	CB-CA-C	-5.83	100.32	111.40
1	B	412	GLY	N-CA-C	5.74	127.45	113.10
1	C	632	LEU	CA-CB-CG	5.07	126.95	115.30

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	487[A]	ARG	Mainchain
1	A	487[B]	ARG	Mainchain
1	B	530[A]	TRP	Mainchain
1	B	530[B]	TRP	Mainchain
1	C	465[B]	GLN	Mainchain
1	D	187[A]	ARG	Mainchain
1	D	187[B]	ARG	Mainchain
1	D	361[A]	ARG	Mainchain
1	D	361[B]	ARG	Mainchain

5.2 Too-close contacts (i)

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	3662	0	3583	67	0
1	B	3641	0	3554	87	0
1	C	3663	0	3571	63	0
1	D	3654	0	3553	96	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	10	0	3	0	0
3	B	10	0	3	0	0
3	C	10	0	3	0	0
3	D	10	0	3	0	0
4	A	4	0	6	0	0
4	B	4	0	6	0	0
4	C	4	0	6	0	0
4	D	4	0	6	0	0
5	A	278	0	0	7	0
5	B	170	0	0	2	0
5	C	236	0	0	2	0
5	D	145	0	0	4	0
All	All	15509	0	14297	288	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 10.

All (288) 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:B:448:VAL:HG23	1:B:451:ARG:HH12	1.34	0.93
1:A:232:ARG:HD2	1:A:394:GLY:O	1.82	0.80
1:C:529:ARG:O	1:C:536:VAL:HG12	1.82	0.79
1:B:515:THR:OG1	1:B:518:GLU:HG3	1.83	0.79
1:B:252:ARG:HH22	1:D:528:ILE:HD13	1.51	0.74
1:D:247:LEU:HA	1:D:250:MET:HE2	1.68	0.73
1:B:410:GLN:HA	1:B:410:GLN:HE21	1.56	0.71
1:B:550:MET:HE1	1:B:598:LEU:HB3	1.72	0.71
1:C:542:LEU:HD22	1:C:546:THR:HG21	1.72	0.70
1:C:436:LEU:HD12	1:D:440[B]:VAL:HG21	1.72	0.70
1:D:436:LEU:O	1:D:440[B]:VAL:HG23	1.91	0.70
1:D:242:PHE:HZ	1:D:250:MET:HE1	1.57	0.70
1:A:232:ARG:HD3	1:A:237:TYR:CD2	2.27	0.69
1:C:232:ARG:HD2	1:C:394:GLY:O	1.93	0.69
1:B:542:LEU:HD23	1:B:542:LEU:H	1.57	0.69
1:A:410:GLN:HE21	1:A:410:GLN:HA	1.57	0.69
1:D:506:ILE:HG23	1:D:570:THR:HG22	1.76	0.66
1:D:410:GLN:HA	1:D:410:GLN:HE21	1.61	0.65
1:B:448:VAL:HG23	1:B:451:ARG:NH1	2.10	0.65
1:A:436:LEU:HD13	1:B:436:LEU:HB3	1.78	0.65
1:B:353:GLY:O	1:B:393:PRO:HD3	1.96	0.65
1:A:280:ARG:HD3	5:A:2053:HOH:O	1.96	0.64
1:C:592:ALA:O	1:C:596:GLU:HG3	1.98	0.64
1:B:435:ILE:HD12	1:B:497:VAL:HG21	1.80	0.64
1:C:465[A]:GLN:HG2	5:C:2160:HOH:O	1.97	0.63
1:C:436:LEU:CD1	1:D:440[B]:VAL:CG2	2.77	0.63
1:C:589:PRO:HD2	1:C:590:GLN:HE22	1.65	0.62
1:D:487:ARG:HD2	5:D:2108:HOH:O	1.99	0.62
1:B:569:TYR:OH	1:B:629:LYS:HE2	1.98	0.62
1:C:232:ARG:HD3	1:C:237:TYR:CD2	2.34	0.62
1:C:353:GLY:O	1:C:393:PRO:HD3	2.00	0.61
1:C:436:LEU:O	1:C:440:VAL:HG23	2.01	0.61
1:D:515:THR:OG1	1:D:518:GLU:HG3	2.00	0.61
1:B:435:ILE:HG12	1:B:492:ALA:HB1	1.83	0.61
1:B:547:GLU:HB2	1:B:635:LYS:HB2	1.82	0.61
1:B:333:ASN:ND2	1:B:411:ASP:HA	2.16	0.61
1:B:335:GLN:HG3	1:B:407:ALA:O	2.02	0.60
1:D:435:ILE:HD11	1:D:494:VAL:HA	1.84	0.60
1:A:534:GLU:OE2	1:C:414:HIS:HD2	1.85	0.59
1:D:335:GLN:HG3	1:D:407:ALA:O	2.03	0.59
1:C:436:LEU:HD12	1:D:440[B]:VAL:CG2	2.33	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:550:MET:HE3	1:C:599:LEU:HD23	1.83	0.59
1:C:542:LEU:HD23	1:C:638:LEU:HD21	1.84	0.59
1:A:195:ILE:HB	1:A:201:ARG:HG2	1.85	0.59
1:A:371:LEU:HG	1:B:451:ARG:HD3	1.85	0.58
1:C:436:LEU:CD1	1:D:440[B]:VAL:HG22	2.33	0.58
1:A:592:ALA:O	1:A:596:GLU:HG3	2.04	0.58
1:B:435:ILE:HD12	1:B:497:VAL:CG2	2.34	0.57
1:B:232:ARG:HD2	1:B:394:GLY:O	2.04	0.57
1:B:542:LEU:HA	1:B:638:LEU:HD11	1.86	0.57
1:D:353:GLY:O	1:D:393:PRO:HD3	2.05	0.57
1:B:413:VAL:HG13	5:B:2084:HOH:O	2.04	0.57
1:C:436:LEU:HD11	1:D:440[B]:VAL:HG22	1.87	0.57
1:A:440:VAL:HG21	1:B:436:LEU:HD12	1.87	0.57
1:A:232:ARG:HD3	1:A:237:TYR:CG	2.41	0.56
1:D:364:ALA:HB1	1:D:365:PRO:HD2	1.87	0.56
1:B:361:ARG:HG3	1:B:386:VAL:HB	1.87	0.56
1:B:275:LEU:O	1:B:277:PRO:HD3	2.05	0.56
1:D:322:MET:HE2	5:D:2075:HOH:O	2.06	0.56
1:D:441:GLN:O	1:D:445:GLU:HG3	2.06	0.56
1:A:220:ARG:HG3	1:A:220:ARG:HH11	1.71	0.55
1:B:514:LEU:HD21	1:B:551:LEU:HD21	1.88	0.55
1:C:436:LEU:HD11	1:D:440[A]:VAL:HG13	1.88	0.55
1:B:451:ARG:HB2	1:B:451:ARG:HH11	1.72	0.55
1:B:530[A]:TRP:CZ3	1:B:535:PRO:HD3	2.40	0.55
1:D:347:PHE:HB2	1:D:420:LEU:HB3	1.88	0.55
1:A:313:ALA:O	1:A:316:GLN:HG2	2.07	0.55
1:B:451:ARG:CB	1:B:451:ARG:HH11	2.20	0.55
1:B:268:ILE:HD11	5:B:2051:HOH:O	2.06	0.55
1:C:440:VAL:HG21	1:D:436:LEU:HD12	1.88	0.54
1:C:550:MET:HE2	1:C:598:LEU:HB3	1.88	0.54
1:B:590:GLN:H	1:B:590:GLN:CD	2.09	0.54
1:D:547:GLU:HB2	1:D:635:LYS:HB2	1.89	0.54
1:A:514:LEU:HD21	1:A:551:LEU:HD21	1.90	0.54
1:D:615:SER:O	1:D:619:GLN:HB2	2.07	0.54
1:B:550:MET:HE1	1:B:598:LEU:CB	2.37	0.53
1:D:352:GLU:HB2	1:D:416:LEU:HB3	1.90	0.53
1:D:341:TYR:CZ	1:D:374:SER:HB3	2.44	0.53
1:D:506:ILE:HG23	1:D:570:THR:CG2	2.39	0.53
1:D:548:VAL:HG12	1:D:634:THR:HG22	1.91	0.52
1:A:341:TYR:CZ	1:A:374:SER:HB3	2.45	0.52
1:B:222:LEU:HD13	1:B:228:VAL:HG21	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:310:GLN:HA	1:B:513:VAL:HG21	1.91	0.52
1:C:255:GLU:OE1	1:C:280:ARG:HD2	2.09	0.52
1:B:267:TYR:C	1:B:268:ILE:HD12	2.30	0.52
1:B:333:ASN:OD1	1:B:411:ASP:HA	2.10	0.52
1:C:275:LEU:HD12	1:C:275:LEU:N	2.25	0.52
1:A:358:ARG:HG2	1:A:388:GLN:HG3	1.92	0.52
1:C:553:ASP:HB2	1:C:602:TYR:CE1	2.44	0.52
1:D:514:LEU:HD21	1:D:551:LEU:HD21	1.92	0.51
1:A:436:LEU:HD11	1:B:488:LEU:HD13	1.92	0.51
1:B:530[B]:TRP:HZ2	1:D:414:HIS:NE2	2.08	0.51
1:A:182:MET:CE	1:A:187:ARG:HH11	2.23	0.51
1:B:333:ASN:CG	1:B:411:ASP:HA	2.30	0.51
1:D:333:ASN:ND2	1:D:411:ASP:HA	2.26	0.51
1:C:515:THR:OG1	1:C:518:GLU:HG3	2.10	0.51
1:C:590:GLN:NE2	1:C:590:GLN:H	2.08	0.51
1:D:363:ARG:NH1	1:D:381:ASP:HB3	2.26	0.51
1:A:354[A]:ARG:CZ	1:A:392:GLU:OE2	2.58	0.51
1:B:363:ARG:NH1	1:B:381:ASP:HB3	2.26	0.51
1:D:613:CYS:SG	1:D:619:GLN:HA	2.50	0.51
1:D:232:ARG:HD3	1:D:394:GLY:O	2.11	0.51
1:C:232:ARG:HD3	1:C:237:TYR:CG	2.46	0.50
1:C:361[A]:ARG:HH11	1:C:361[A]:ARG:HG2	1.75	0.50
1:D:301:PRO:HG2	1:D:327:VAL:HG23	1.93	0.50
1:A:410:GLN:NE2	1:A:410:GLN:HA	2.24	0.50
1:B:232:ARG:HD3	1:B:237:TYR:CD2	2.46	0.50
1:D:275:LEU:N	1:D:275:LEU:HD12	2.26	0.50
1:B:436:LEU:O	1:B:440[B]:VAL:HG23	2.12	0.50
1:D:363:ARG:HB2	1:D:367:GLU:OE1	2.11	0.50
1:B:622:LEU:O	1:B:626:LEU:HG	2.10	0.50
1:B:569:TYR:CZ	1:B:629:LYS:HE2	2.47	0.50
1:B:341:TYR:CZ	1:B:374:SER:HB3	2.46	0.50
1:B:550:MET:HE3	1:B:599:LEU:HD23	1.92	0.50
1:D:315:LEU:CD1	1:D:420:LEU:HD11	2.42	0.49
1:A:436:LEU:HD11	1:B:488:LEU:CD1	2.43	0.49
1:B:333:ASN:HD21	1:B:411:ASP:HA	1.78	0.49
1:B:530[B]:TRP:CZ2	1:D:414:HIS:NE2	2.80	0.49
1:B:548:VAL:HG21	1:B:632:LEU:HD21	1.94	0.49
1:B:358:ARG:HG2	1:B:388:GLN:HG3	1.94	0.49
1:D:530:TRP:CZ3	1:D:535:PRO:HD3	2.48	0.49
1:A:633:LEU:HD12	1:A:633:LEU:C	2.33	0.49
1:B:633:LEU:HD12	1:B:633:LEU:C	2.33	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:188:VAL:O	1:B:192:LEU:HG	2.13	0.48
1:A:352:GLU:HB2	1:A:416:LEU:HB3	1.95	0.48
1:A:441:GLN:O	1:A:445:GLU:HG3	2.13	0.48
1:D:435:ILE:HG13	1:D:497:VAL:HG21	1.95	0.48
5:A:2191:HOH:O	1:B:482[B]:ARG:HG3	2.12	0.48
1:A:409:CYS:SG	1:A:415:SER:HB3	2.54	0.48
1:C:333:ASN:OD1	1:C:411:ASP:HA	2.13	0.48
1:C:420:LEU:C	1:C:420:LEU:HD23	2.33	0.48
1:D:555:ILE:O	1:D:569:TYR:HA	2.14	0.48
1:D:247:LEU:HA	1:D:250:MET:CE	2.40	0.48
1:D:436:LEU:O	1:D:440[A]:VAL:HG22	2.14	0.48
1:B:275:LEU:HD12	1:B:275:LEU:N	2.29	0.48
1:B:187:ARG:HH11	1:B:187:ARG:HG2	1.79	0.48
1:A:341:TYR:CE1	1:A:374:SER:HB3	2.49	0.48
1:B:568:TYR:CD2	1:B:584:CYS:HB3	2.48	0.48
1:D:359:VAL:O	1:D:386:VAL:HG12	2.14	0.48
1:A:275:LEU:HD12	1:A:275:LEU:N	2.29	0.48
1:C:297:ARG:HD3	1:C:328:TYR:CE2	2.49	0.48
1:D:266:ARG:O	1:D:273:GLU:HG2	2.14	0.47
1:D:345:GLU:OE2	1:D:401:ARG:HG2	2.13	0.47
1:A:487[A]:ARG:NH1	5:A:2159:HOH:O	2.47	0.47
1:D:386:VAL:O	1:D:386:VAL:HG22	2.14	0.47
1:A:250:MET:HE1	1:A:298:LEU:HD21	1.95	0.47
1:A:275:LEU:O	1:A:277:PRO:HD3	2.14	0.47
1:D:447:ASN:HD22	1:D:449:GLU:H	1.62	0.47
1:A:418:LEU:C	1:A:418:LEU:HD23	2.34	0.47
1:A:297:ARG:HD3	1:A:328:TYR:CE2	2.49	0.47
1:D:609:GLY:HA2	1:D:619:GLN:OE1	2.14	0.47
1:C:527:PRO:O	1:C:528:ILE:HD13	2.14	0.47
1:A:333:ASN:ND2	1:A:411:ASP:HA	2.30	0.47
1:B:633:LEU:O	1:B:633:LEU:HD12	2.15	0.47
1:B:265:ALA:HB1	1:B:272:ARG:HE	1.79	0.47
1:D:536:VAL:HG12	1:D:536:VAL:O	2.15	0.47
1:C:590:GLN:CD	1:C:590:GLN:H	2.18	0.46
1:D:459:MET:HG3	5:D:2091:HOH:O	2.15	0.46
1:D:361[A]:ARG:HG3	1:D:386:VAL:HB	1.97	0.46
1:D:298:LEU:HD23	1:D:301:PRO:HG3	1.97	0.46
1:D:275:LEU:O	1:D:277:PRO:HD3	2.15	0.46
1:D:257:GLN:HE22	1:D:280:ARG:HB2	1.81	0.46
1:D:553:ASP:HB2	1:D:602:TYR:CE1	2.51	0.46
1:C:197:SER:O	1:C:201:ARG:HG3	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:374:SER:HB2	1:D:375:PRO:HD2	1.98	0.46
1:B:374:SER:HB2	1:B:375:PRO:HD2	1.98	0.46
1:A:192:LEU:O	1:A:201:ARG:HD3	2.15	0.46
1:A:536:VAL:HG23	1:A:536:VAL:O	2.15	0.46
1:A:333:ASN:OD1	1:A:411:ASP:HA	2.15	0.45
1:B:531:GLU:O	1:B:532:ALA:HB3	2.16	0.45
1:D:246:ASP:O	1:D:250:MET:HG3	2.16	0.45
1:C:506:ILE:HG23	1:C:570:THR:HG22	1.98	0.45
1:C:183:SER:CB	1:C:239:GLN:HB3	2.46	0.45
1:A:300:CYS:SG	5:A:2084:HOH:O	2.61	0.45
1:A:344:ILE:O	1:A:344:ILE:HD12	2.16	0.45
1:C:589:PRO:HD2	1:C:590:GLN:NE2	2.31	0.45
1:A:182:MET:HE3	1:A:187:ARG:HH11	1.81	0.45
1:C:250:MET:HE1	1:C:298:LEU:HD21	1.98	0.45
1:B:565:LEU:HB2	1:B:587:ILE:O	2.17	0.45
1:D:195:ILE:HB	1:D:201:ARG:HG2	1.99	0.45
1:B:544:THR:HA	1:B:608:VAL:HB	1.98	0.45
1:A:310:GLN:HA	1:A:513:VAL:HG21	1.99	0.45
1:A:501:ARG:HD2	5:A:2149:HOH:O	2.15	0.45
1:B:530[A]:TRP:CZ2	1:D:244:THR:HG21	2.51	0.45
1:D:399:PHE:HA	1:D:400:PRO:HD3	1.79	0.45
1:A:531:GLU:O	1:A:532:ALA:HB3	2.17	0.45
1:B:341:TYR:CE2	1:B:374:SER:HB3	2.52	0.44
1:B:185:LEU:O	1:B:188:VAL:HG12	2.17	0.44
1:A:568:TYR:CD2	1:A:584:CYS:HB3	2.53	0.44
1:B:410:GLN:NE2	1:B:410:GLN:HA	2.30	0.44
1:B:214:PRO:HA	1:B:215:PRO:HD3	1.87	0.44
1:C:536:VAL:HG22	1:C:537:ASN:N	2.32	0.44
1:B:542:LEU:HD21	1:B:624:THR:OG1	2.17	0.44
1:D:529:ARG:H	1:D:537:ASN:CB	2.31	0.44
1:C:640:LEU:HD23	1:C:640:LEU:H	1.81	0.44
1:D:480:LYS:O	1:D:483:VAL:HG12	2.17	0.44
1:C:436:LEU:HD11	1:D:440[A]:VAL:CG1	2.47	0.44
1:D:528:ILE:HD12	1:D:528:ILE:N	2.32	0.44
1:B:546:THR:O	1:B:607:ARG:HA	2.18	0.44
1:B:537:ASN:CB	1:D:291:GLN:HE22	2.31	0.44
1:B:432:LEU:HA	1:B:435:ILE:HG22	2.00	0.44
1:A:275:LEU:HD22	1:A:294:CYS:SG	2.58	0.44
1:C:360:TYR:CE2	1:C:385:PRO:HG3	2.53	0.44
1:A:515:THR:OG1	1:A:518:GLU:HG3	2.17	0.44
1:D:287:TRP:O	1:D:291:GLN:HG3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:197:SER:O	1:B:201:ARG:HG3	2.18	0.44
1:D:633:LEU:HD12	1:D:633:LEU:C	2.38	0.43
1:A:436:LEU:O	1:A:440:VAL:HG23	2.17	0.43
1:C:195:ILE:HB	1:C:201:ARG:HG2	1.99	0.43
1:C:187:ARG:NH1	1:C:187:ARG:HB2	2.34	0.43
1:D:297:ARG:HD3	1:D:328:TYR:CE2	2.52	0.43
1:A:404:ILE:HG13	5:A:2125:HOH:O	2.18	0.43
1:A:315:LEU:CD1	1:A:420:LEU:HD11	2.48	0.43
1:A:590:GLN:H	1:A:590:GLN:CD	2.20	0.43
1:D:333:ASN:OD1	1:D:411:ASP:HA	2.19	0.43
1:D:418:LEU:C	1:D:418:LEU:HD23	2.39	0.43
1:C:341:TYR:CZ	1:C:374:SER:HB3	2.54	0.43
1:B:451:ARG:HB2	1:B:451:ARG:NH1	2.34	0.43
1:B:195:ILE:HA	1:B:196:PRO:HD3	1.89	0.43
1:A:386:VAL:HG22	1:A:386:VAL:O	2.18	0.43
1:B:435:ILE:HD11	1:B:494:VAL:HA	2.01	0.43
1:D:344:ILE:CG2	1:D:424:GLN:HB2	2.48	0.43
1:C:633:LEU:HD12	1:C:633:LEU:C	2.38	0.43
1:A:252:ARG:NH1	5:A:2055:HOH:O	2.51	0.43
1:D:363:ARG:HH12	1:D:381:ASP:HB3	1.84	0.43
1:C:503:LYS:HE3	1:C:568:TYR:CZ	2.54	0.43
1:D:333:ASN:CG	1:D:411:ASP:HA	2.39	0.42
1:D:231:ARG:NH2	1:D:389:THR:OG1	2.51	0.42
1:D:531:GLU:O	1:D:532:ALA:HB3	2.19	0.42
1:C:345:GLU:OE2	1:C:401:ARG:HG2	2.19	0.42
1:D:252:ARG:HG3	1:D:252:ARG:HH11	1.83	0.42
1:A:436:LEU:HD12	1:B:440[B]:VAL:CG2	2.49	0.42
1:D:384:GLU:HA	1:D:385:PRO:HD3	1.93	0.42
1:A:530:TRP:CZ3	1:A:535:PRO:HD3	2.53	0.42
1:A:545:GLU:HG3	1:A:607:ARG:NH2	2.33	0.42
1:C:485:VAL:O	1:C:488:LEU:HB2	2.19	0.42
1:A:440:VAL:CG2	1:B:436:LEU:HD12	2.48	0.42
1:B:550:MET:HE3	1:B:599:LEU:CD2	2.48	0.42
1:C:488:LEU:HD11	1:D:436:LEU:HD11	2.00	0.42
1:A:216:ASP:OD2	1:A:220:ARG:NH2	2.51	0.42
1:C:333:ASN:CG	1:C:411:ASP:HA	2.40	0.42
1:C:335:GLN:HG3	1:C:407:ALA:O	2.19	0.42
1:C:589:PRO:HB2	1:C:590:GLN:HE21	1.85	0.42
1:A:542:LEU:N	1:A:542:LEU:HD12	2.35	0.42
1:B:359:VAL:O	1:B:386:VAL:HG12	2.20	0.42
1:A:213:MET:HA	1:A:214:PRO:HD3	1.92	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:272:ARG:HG3	1:A:272:ARG:HH11	1.84	0.42
1:D:527:PRO:HD2	1:D:639:ALA:HB3	2.02	0.42
1:D:468:ASP:HB2	5:D:2099:HOH:O	2.20	0.42
1:B:315:LEU:CD1	1:B:420:LEU:HD11	2.49	0.42
1:C:192:LEU:O	1:C:201:ARG:HD3	2.18	0.41
1:D:360:TYR:CE2	1:D:385:PRO:HG3	2.55	0.41
1:D:298:LEU:HB3	1:D:327:VAL:HB	2.01	0.41
1:A:244:THR:HG21	1:C:530:TRP:CE2	2.55	0.41
1:B:542:LEU:H	1:B:542:LEU:CD2	2.28	0.41
1:A:217:HIS:ND1	1:A:221:ARG:HD3	2.35	0.41
1:A:214:PRO:HA	1:A:215:PRO:HD3	1.94	0.41
1:D:565:LEU:HB2	1:D:587:ILE:O	2.21	0.41
1:D:546:THR:O	1:D:607:ARG:HA	2.20	0.41
1:B:266:ARG:HG3	1:B:268:ILE:HD13	2.03	0.41
1:A:325:SER:HA	1:A:419:THR:O	2.20	0.41
1:C:550:MET:HE2	1:C:598:LEU:C	2.41	0.41
1:D:548:VAL:HG21	1:D:632:LEU:HD21	2.03	0.41
1:B:549:HIS:C	1:B:632:LEU:HD12	2.42	0.41
1:B:549:HIS:CE1	1:B:633:LEU:HD11	2.56	0.41
1:B:553:ASP:HB2	1:B:602:TYR:CE1	2.56	0.41
1:A:291:GLN:HE22	1:C:538:VAL:CB	2.34	0.41
1:C:373:SER:HB3	5:C:2096:HOH:O	2.21	0.41
1:D:221:ARG:O	1:D:225:ARG:HD2	2.20	0.41
1:C:550:MET:CE	1:C:598:LEU:HB3	2.50	0.41
1:C:272:ARG:HH11	1:C:272:ARG:HG3	1.85	0.41
1:D:301:PRO:HB2	1:D:308:VAL:HG11	2.03	0.40
1:D:214:PRO:HA	1:D:215:PRO:HD3	1.95	0.40
1:B:232:ARG:HD3	1:B:237:TYR:CG	2.55	0.40
1:C:553:ASP:HB2	1:C:602:TYR:CD1	2.56	0.40
1:C:526:LEU:HG	1:C:528:ILE:HD11	2.03	0.40
1:A:382:LEU:HD22	1:A:404:ILE:HG21	2.04	0.40
1:B:287:TRP:HA	1:B:287:TRP:CE3	2.57	0.40
1:A:399:PHE:HA	1:A:400:PRO:HD3	1.86	0.40
1:D:310:GLN:HA	1:D:513:VAL:HG21	2.03	0.40
1:D:410:GLN:HA	1:D:410:GLN:NE2	2.32	0.40
1:C:429:GLY:O	1:C:433:GLU:HG3	2.22	0.40
1:C:440:VAL:CG2	1:D:436:LEU:CD1	2.99	0.40
1:B:267:TYR:CZ	1:B:270:GLY:HA2	2.57	0.40
1:D:568:TYR:CD2	1:D:584:CYS:HB3	2.57	0.40
1:D:223:TRP:CD1	1:D:224:GLU:HG3	2.57	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	454/467 (97%)	446 (98%)	8 (2%)	0	100	100
1	B	456/467 (98%)	442 (97%)	14 (3%)	0	100	100
1	C	458/467 (98%)	450 (98%)	8 (2%)	0	100	100
1	D	458/467 (98%)	443 (97%)	15 (3%)	0	100	100
All	All	1826/1868 (98%)	1781 (98%)	45 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	388/399 (97%)	382 (98%)	6 (2%)	72	78
1	B	382/399 (96%)	369 (97%)	13 (3%)	44	42
1	C	386/399 (97%)	379 (98%)	7 (2%)	66	71
1	D	383/399 (96%)	371 (97%)	12 (3%)	47	47
All	All	1539/1596 (96%)	1501 (98%)	38 (2%)	60	58

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	194	ARG
1	A	232	ARG

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Mol	Chain	Res	Type
1	A	280	ARG
1	A	468	ASP
1	A	590	GLN
1	A	603	PRO
1	B	187	ARG
1	B	232	ARG
1	B	233	GLN
1	B	280	ARG
1	B	410	GLN
1	B	420	LEU
1	B	435	ILE
1	B	451	ARG
1	B	530[A]	TRP
1	B	530[B]	TRP
1	B	550	MET
1	B	590	GLN
1	B	607	ARG
1	C	232	ARG
1	C	255	GLU
1	C	410	GLN
1	C	517[A]	ARG
1	C	517[B]	ARG
1	C	534	GLU
1	C	603	PRO
1	D	187[A]	ARG
1	D	187[B]	ARG
1	D	194	ARG
1	D	232	ARG
1	D	410	GLN
1	D	435	ILE
1	D	440[A]	VAL
1	D	440[B]	VAL
1	D	447	ASN
1	D	468	ASP
1	D	580	GLU
1	D	636	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	239	GLN
1	A	257	GLN

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Mol	Chain	Res	Type
1	A	291	GLN
1	A	410	GLN
1	A	500	GLN
1	A	537	ASN
1	B	257	GLN
1	B	326	ASN
1	B	410	GLN
1	B	424	GLN
1	B	590	GLN
1	C	318	GLN
1	C	414	HIS
1	C	424	GLN
1	C	590	GLN
1	D	257	GLN
1	D	291	GLN
1	D	379	GLN
1	D	406	GLN
1	D	410	GLN
1	D	447	ASN
1	D	500	GLN
1	D	590	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 12 ligands modelled in this entry, 4 are monoatomic - leaving 8 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	OGA	A	902	2	3,9,9	0.39	0	3,11,11	0.51	0
4	EDO	A	903	-	3,3,3	0.50	0	2,2,2	0.36	0
3	OGA	B	902	2	3,9,9	0.43	0	3,11,11	0.51	0
4	EDO	B	903	-	3,3,3	0.44	0	2,2,2	0.43	0
3	OGA	C	902	2	3,9,9	0.41	0	3,11,11	0.51	0
4	EDO	C	903	-	3,3,3	0.43	0	2,2,2	0.43	0
3	OGA	D	902	2	3,9,9	0.44	0	3,11,11	0.51	0
4	EDO	D	903	-	3,3,3	0.45	0	2,2,2	0.43	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
3	OGA	A	902	2	-	0/3/9/9	0/0/0/0
4	EDO	A	903	-	-	0/1/1/1	0/0/0/0
3	OGA	B	902	2	-	0/3/9/9	0/0/0/0
4	EDO	B	903	-	-	0/1/1/1	0/0/0/0
3	OGA	C	902	2	-	0/3/9/9	0/0/0/0
4	EDO	C	903	-	-	0/1/1/1	0/0/0/0
3	OGA	D	902	2	-	0/3/9/9	0/0/0/0
4	EDO	D	903	-	-	0/1/1/1	0/0/0/0

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

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	456/467 (97%)	-0.01	2 (0%) 93 94	22, 34, 58, 78	1 (0%)
1	B	456/467 (97%)	0.12	13 (2%) 55 65	22, 41, 86, 100	3 (0%)
1	C	458/467 (98%)	-0.02	10 (2%) 65 73	23, 36, 63, 93	2 (0%)
1	D	459/467 (98%)	0.08	7 (1%) 76 82	24, 46, 80, 100	0
All	All	1829/1868 (97%)	0.04	32 (1%) 73 80	22, 39, 74, 100	6 (0%)

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	530[A]	TRP	11.4
1	C	528	ILE	7.4
1	B	536	VAL	5.8
1	C	530	TRP	4.8
1	B	532	ALA	4.5
1	C	640	LEU	3.9
1	D	538	VAL	3.9
1	C	537	ASN	3.9
1	C	532	ALA	3.8
1	B	614	ASP	3.5
1	D	641	ASN	3.5
1	D	528	ILE	3.2
1	D	540	ALA	3.1
1	B	620	LEU	3.0
1	C	639	ALA	2.8
1	B	613	CYS	2.8
1	A	639	ALA	2.6
1	B	617	GLU	2.6
1	B	588	TYR	2.6
1	B	562	GLY	2.5
1	C	535	PRO	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	520	ALA	2.4
1	D	636	MET	2.3
1	B	531	GLU	2.3
1	B	547	GLU	2.2
1	A	529	ARG	2.2
1	B	608	VAL	2.2
1	D	537	ASN	2.2
1	C	411	ASP	2.1
1	C	468[A]	ASP	2.1
1	C	536	VAL	2.1
1	D	361[A]	ARG	2.1

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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
4	EDO	B	903	4/4	0.98	0.16	5.69	32,37,38,42	0
4	EDO	C	903	4/4	0.96	0.14	2.86	34,35,35,37	0
4	EDO	D	903	4/4	0.96	0.13	2.72	50,51,52,52	0
3	OGA	D	902	10/10	0.94	0.12	-0.08	52,54,57,57	0
4	EDO	A	903	4/4	0.98	0.11	-0.14	31,35,36,37	0
3	OGA	C	902	10/10	0.95	0.10	-0.66	38,40,46,47	0
3	OGA	B	902	10/10	0.94	0.10	-1.02	37,43,47,48	0
3	OGA	A	902	10/10	0.96	0.10	-1.33	36,41,43,45	0
2	MN	D	901	1/1	1.00	0.21	-	28,28,28,28	0
2	MN	C	901	1/1	1.00	0.21	-	20,20,20,20	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	MN	A	901	1/1	1.00	0.22	-	18,18,18,18	0
2	MN	B	901	1/1	1.00	0.20	-	18,18,18,18	0

6.5 Other polymers (i)

There are no such residues in this entry.