Full wwPDB X-ray Structure Validation Report (i)

Mar 10, 2024 – 01:14 AM EST

PDB ID	:	4E4H
Title	:	Crystal structure of Histone Demethylase NO66
Authors	:	Wu, M.; Tao, Y.; Zang, J.
Deposited on	:	2012-03-13
Resolution	:	2.28 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

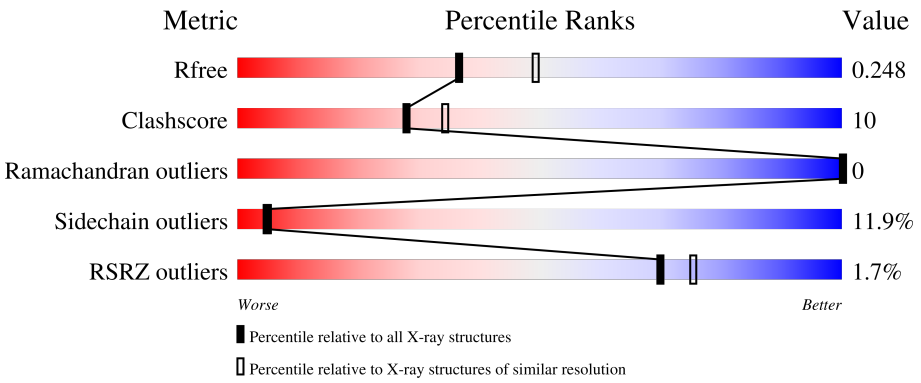
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.28 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	6980 (2.30-2.26)
Clashscore	141614	7711 (2.30-2.26)
Ramachandran outliers	138981	7597 (2.30-2.26)
Sidechain outliers	138945	7598 (2.30-2.26)
RSRZ outliers	127900	6849 (2.30-2.26)

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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	463	.% 73% 22% • •
1	B	463	2% 75% 20% • •
1	C	463	73% 21% • • •
1	D	463	3% 74% 21% • •

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
5	PEG	C	1003	-	-	X	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 15448 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 Lysine-specific demethylase NO66.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	455	3692	2348	652	676	16	0	7	0
1	B	458	3744	2381	659	686	18	0	13	0
1	C	455	3696	2348	655	677	16	0	7	0
1	D	457	3706	2356	653	681	16	0	7	0

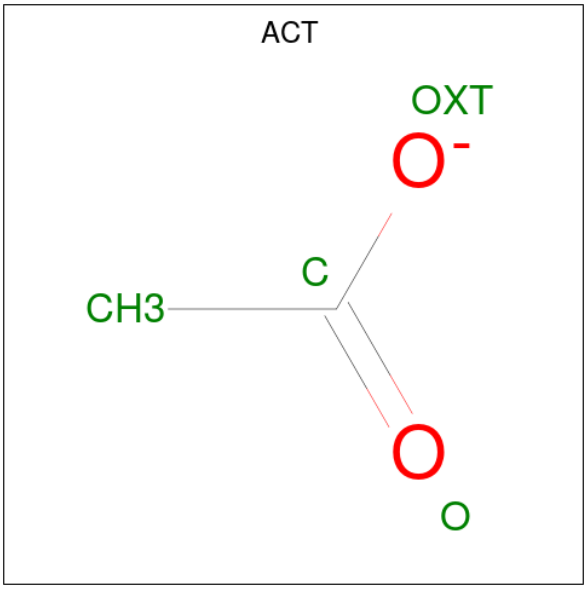
There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	179	HIS	-	expression tag	UNP Q9H6W3
A	180	MET	-	expression tag	UNP Q9H6W3
A	181	GLY	-	expression tag	UNP Q9H6W3
A	182	SER	-	expression tag	UNP Q9H6W3
A	364	ALA	VAL	SEE REMARK 999	UNP Q9H6W3
B	179	HIS	-	expression tag	UNP Q9H6W3
B	180	MET	-	expression tag	UNP Q9H6W3
B	181	GLY	-	expression tag	UNP Q9H6W3
B	182	SER	-	expression tag	UNP Q9H6W3
B	364	ALA	VAL	SEE REMARK 999	UNP Q9H6W3
C	179	HIS	-	expression tag	UNP Q9H6W3
C	180	MET	-	expression tag	UNP Q9H6W3
C	181	GLY	-	expression tag	UNP Q9H6W3
C	182	SER	-	expression tag	UNP Q9H6W3
C	364	ALA	VAL	SEE REMARK 999	UNP Q9H6W3
D	179	HIS	-	expression tag	UNP Q9H6W3
D	180	MET	-	expression tag	UNP Q9H6W3
D	181	GLY	-	expression tag	UNP Q9H6W3
D	182	SER	-	expression tag	UNP Q9H6W3
D	364	ALA	VAL	SEE REMARK 999	UNP Q9H6W3

- Molecule 2 is FE (III) ION (three-letter code: FE) (formula: Fe).

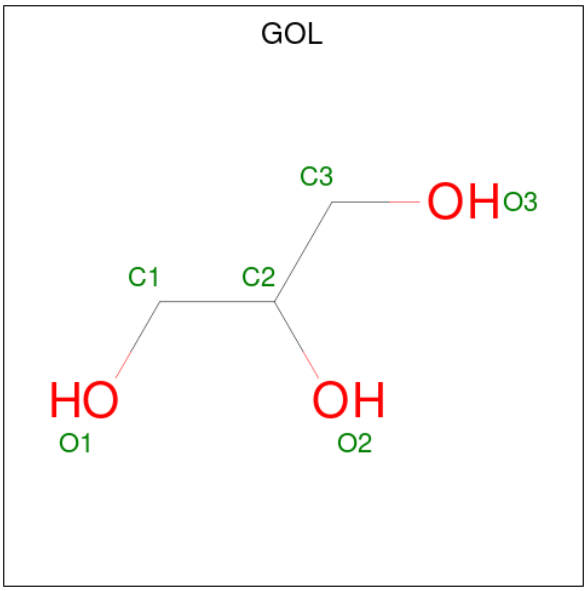
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Fe		
2	A	1	1	1	0	0
2	B	1	1	1	0	0
2	C	1	1	1	0	0
2	D	1	1	1	0	0

- Molecule 3 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



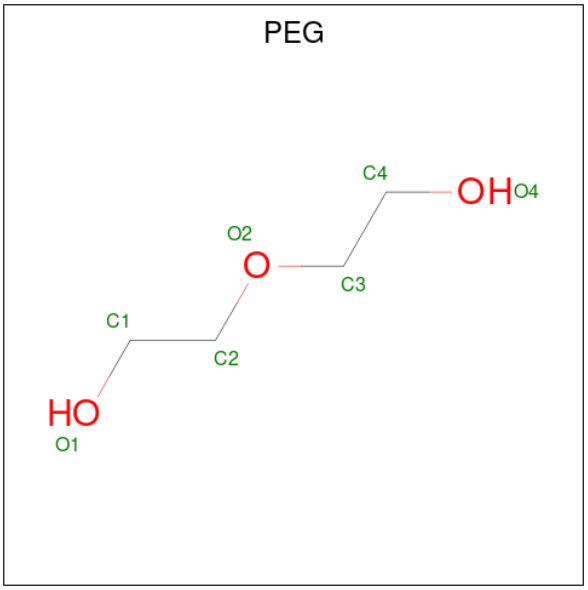
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
3	A	1	4	2	2	0	0

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
4	C	1	6	3	3	0	0

- Molecule 5 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
5	C	1	7	4	3	0	0

- Molecule 6 is water.

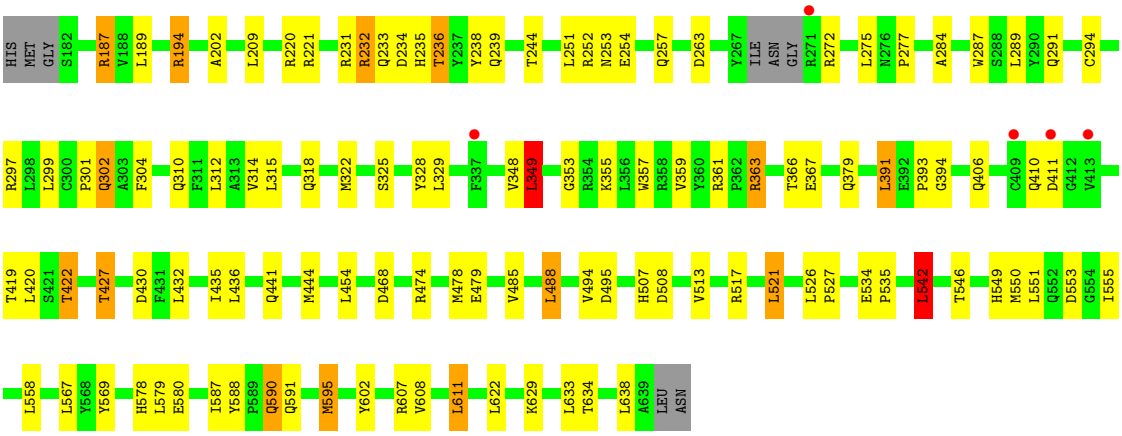
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	144	144	144	0	0
			Total	O		
6	B	148	148	148	0	0
			Total	O		
6	C	167	167	167	0	0
			Total	O		
6	D	130	130	130	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

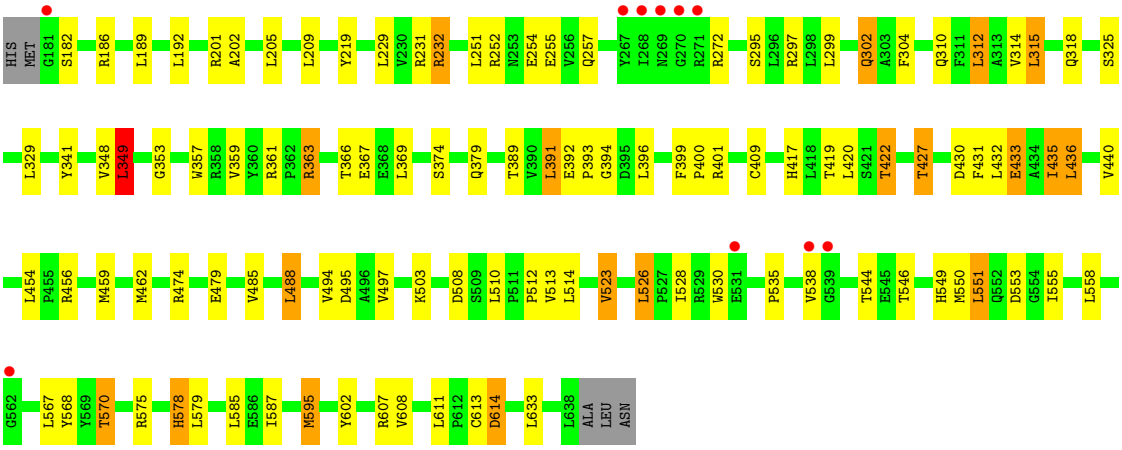
• Molecule 1: Lysine-specific demethylase NO66

Chain A:



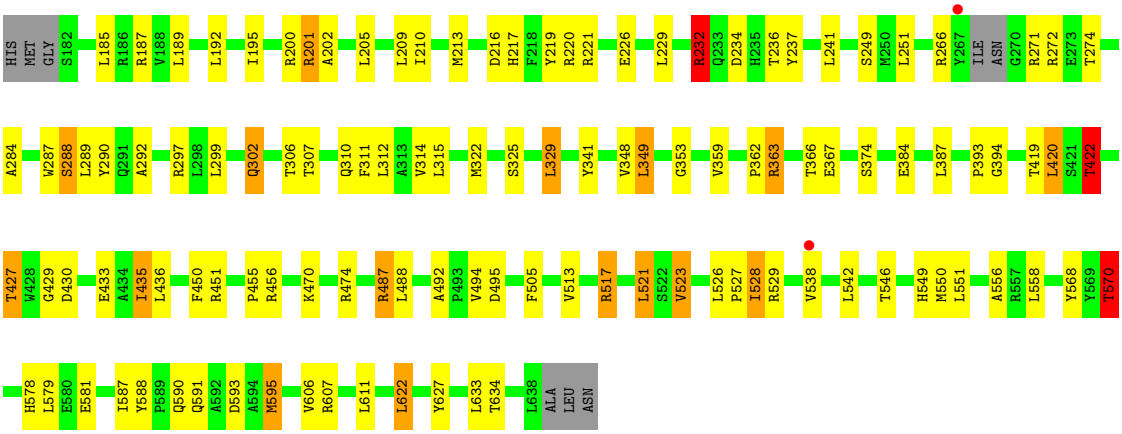
• Molecule 1: Lysine-specific demethylase NO66

Chain B:



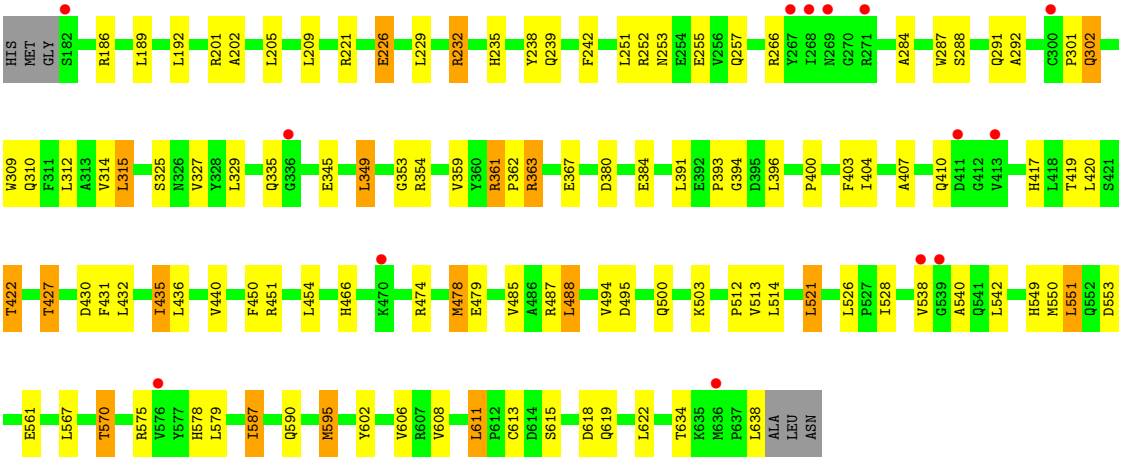
• Molecule 1: Lysine-specific demethylase NO66

Chain C:



• Molecule 1: Lysine-specific demethylase NO66

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α, β, γ	89.35Å 89.35Å 304.86Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 2.28 44.20 – 2.28	Depositor EDS
% Data completeness (in resolution range)	98.8 (50.00-2.28) 98.9 (44.20-2.28)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.23 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.202 , 0.252 0.198 , 0.248	Depositor DCC
R_{free} test set	6135 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	40.8	Xtriage
Anisotropy	0.093	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 31.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.000 for -h,-k,l 0.028 for h,-h-k,-l 0.017 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	15448	wwPDB-VP
Average B, all atoms (Å^2)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.46% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: ACT, GOL, FE, PEG

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	0.63	0/3807	0.76	4/5178 (0.1%)
1	B	0.63	0/3882	0.76	3/5281 (0.1%)
1	C	0.65	0/3811	0.84	9/5181 (0.2%)
1	D	0.60	0/3822	0.75	5/5201 (0.1%)
All	All	0.63	0/15322	0.78	21/20841 (0.1%)

There are no bond length outliers.

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	451	ARG	NE-CZ-NH2	-11.40	114.60	120.30
1	C	232	ARG	NE-CZ-NH2	-9.49	115.55	120.30
1	D	451	ARG	NE-CZ-NH2	-8.51	116.04	120.30
1	C	451	ARG	NE-CZ-NH1	8.08	124.34	120.30
1	A	420	LEU	CA-CB-CG	6.54	130.35	115.30
1	B	551	LEU	CA-CB-CG	6.42	130.08	115.30
1	A	595	MET	CG-SD-CE	6.16	110.06	100.20
1	A	349	LEU	CA-CB-CG	6.09	129.31	115.30
1	C	201	ARG	NE-CZ-NH2	-6.09	117.25	120.30
1	C	349	LEU	CA-CB-CG	5.77	128.57	115.30
1	B	349	LEU	CA-CB-CG	5.61	128.19	115.30
1	C	422	THR	CB-CA-C	-5.60	96.48	111.60
1	C	187	ARG	NE-CZ-NH1	5.50	123.05	120.30
1	D	422	THR	CB-CA-C	-5.37	97.11	111.60
1	D	551	LEU	CA-CB-CG	5.31	127.52	115.30
1	D	451	ARG	NE-CZ-NH1	5.25	122.93	120.30
1	D	595	MET	CG-SD-CE	5.13	108.40	100.20
1	C	570	THR	N-CA-CB	-5.10	100.62	110.30
1	C	420	LEU	CA-CB-CG	5.08	126.99	115.30
1	A	542	LEU	CA-CB-CG	5.08	126.98	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	422	THR	CB-CA-C	-5.07	97.90	111.60

There are no chirality outliers.

There are no planarity outliers.

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	3692	0	3630	71	0
1	B	3744	0	3692	83	0
1	C	3696	0	3629	95	0
1	D	3706	0	3641	72	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	4	0	3	0	0
4	C	6	0	8	3	0
5	C	7	0	10	8	0
6	A	144	0	0	1	0
6	B	148	0	0	5	0
6	C	167	0	0	7	0
6	D	130	0	0	6	0
All	All	15448	0	14613	293	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 (293) 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:C:200[B]:ARG:CG	1:C:200[B]:ARG:HH11	1.60	1.15
1:C:271:ARG:HG2	1:C:272:ARG:H	1.21	1.05
1:A:302:GLN:H	1:A:302:GLN:HE21	1.02	0.98
1:C:200[B]:ARG:HH11	1:C:200[B]:ARG:HG3	1.26	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:236:THR:HG21	6:C:1251:HOH:O	1.66	0.94
1:C:487[A]:ARG:CB	1:C:487[A]:ARG:HH11	1.81	0.93
1:D:302:GLN:HE21	1:D:302:GLN:H	1.18	0.92
1:B:526:LEU:HD13	1:B:528:ILE:HG12	1.52	0.91
1:B:435:ILE:HD11	1:B:494:VAL:HA	1.54	0.88
1:C:200[B]:ARG:CG	1:C:200[B]:ARG:NH1	2.33	0.87
1:B:254:GLU:HG2	1:B:304:PHE:CD1	2.12	0.85
1:C:200[B]:ARG:HH11	1:C:200[B]:ARG:HG2	1.40	0.84
1:D:521:LEU:HG	1:D:634:THR:O	1.79	0.83
1:C:587:ILE:HD13	1:C:595:MET:HG3	1.60	0.83
1:C:487[A]:ARG:HH11	1:C:487[A]:ARG:CG	1.92	0.82
1:B:302:GLN:H	1:B:302:GLN:HE21	1.27	0.82
1:A:291:GLN:HG3	1:B:538:VAL:HG11	1.61	0.81
1:B:427:THR:HB	1:B:430:ASP:OD2	1.81	0.80
1:D:427:THR:HB	1:D:430:ASP:OD2	1.81	0.80
1:A:427:THR:HG22	1:A:430:ASP:H	1.47	0.79
1:B:427:THR:HG22	1:B:430:ASP:H	1.47	0.79
1:C:302:GLN:H	1:C:302:GLN:HE21	1.30	0.79
1:D:570:THR:HG21	6:D:1128:HOH:O	1.83	0.77
1:D:427:THR:HG22	1:D:430:ASP:H	1.48	0.77
1:B:363:ARG:HG2	1:B:367:GLU:OE1	1.86	0.75
1:D:431:PHE:CE2	1:D:435:ILE:HD12	2.22	0.75
1:A:567:LEU:HB2	1:A:587:ILE:CD1	2.16	0.75
1:B:440:VAL:HG21	1:C:436:LEU:HD12	1.70	0.74
1:D:542:LEU:HD23	1:D:638:LEU:HD11	1.70	0.74
1:C:232:ARG:HD2	1:C:394:GLY:O	1.88	0.72
1:A:427:THR:HB	1:A:430:ASP:OD2	1.88	0.72
1:A:410:GLN:HB3	1:A:411:ASP:OD2	1.90	0.72
1:B:459:MET:CE	4:C:1002:GOL:H12	2.21	0.71
1:B:353:GLY:O	1:B:393:PRO:HD3	1.91	0.71
1:A:494[B]:VAL:HG21	1:D:478:MET:SD	2.32	0.70
1:A:275:LEU:HD13	1:A:294:CYS:SG	2.31	0.70
1:A:590:GLN:NE2	1:A:590:GLN:H	1.90	0.70
1:A:436:LEU:HD22	1:D:436:LEU:HD22	1.73	0.69
1:D:232:ARG:HD3	1:D:394:GLY:O	1.91	0.69
1:B:297:ARG:HE	1:B:299:LEU:HD21	1.57	0.69
1:C:202:ALA:HA	1:C:314:VAL:HG23	1.76	0.68
1:D:500:GLN:OE1	1:D:503:LYS:HE2	1.93	0.68
1:B:436:LEU:HD11	1:C:488:LEU:HD23	1.75	0.68
1:C:297:ARG:HH21	1:C:299:LEU:HD21	1.59	0.68
1:C:200[B]:ARG:HG3	1:C:200[B]:ARG:NH1	2.01	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:455:PRO:HB3	5:C:1003:PEG:H21	1.76	0.67
1:C:549:HIS:HD2	1:C:550:MET:O	1.77	0.67
1:C:271:ARG:HG2	1:C:272:ARG:N	2.03	0.67
1:A:302:GLN:H	1:A:302:GLN:NE2	1.84	0.66
1:A:254:GLU:HG2	1:A:304:PHE:CD1	2.30	0.66
1:B:357:TRP:CD1	1:B:391:LEU:HD22	2.31	0.66
1:C:456:ARG:HE	5:C:1003:PEG:H42	1.60	0.66
1:C:200[B]:ARG:NH1	1:C:200[B]:ARG:HG2	2.05	0.66
1:A:302:GLN:HE21	1:A:302:GLN:N	1.86	0.66
1:C:427:THR:HB	1:C:430:ASP:OD2	1.96	0.65
1:D:310:GLN:HA	1:D:513:VAL:HG21	1.77	0.65
1:B:526:LEU:HD13	1:B:528:ILE:CG1	2.24	0.65
1:D:435:ILE:HD11	1:D:494:VAL:HA	1.79	0.65
1:B:587:ILE:HG12	1:B:595:MET:HG3	1.79	0.65
1:D:302:GLN:H	1:D:302:GLN:NE2	1.90	0.65
1:C:353:GLY:O	1:C:393:PRO:HD3	1.97	0.65
1:C:487[A]:ARG:HH11	1:C:487[A]:ARG:HB3	1.62	0.64
1:B:570:THR:HG21	6:B:1126:HOH:O	1.97	0.64
1:A:297:ARG:HD2	1:A:328:TYR:CE1	2.33	0.64
1:A:220:ARG:HG3	1:A:221:ARG:HG2	1.79	0.63
1:B:440:VAL:CG2	1:C:436:LEU:CD1	2.77	0.62
1:C:523:VAL:HG23	6:C:1124:HOH:O	1.99	0.62
1:C:570:THR:HG21	6:C:1109:HOH:O	1.98	0.62
1:D:542:LEU:CD2	1:D:638:LEU:HD11	2.29	0.62
1:C:427:THR:HG22	1:C:430:ASP:H	1.64	0.62
1:B:192:LEU:HG	1:B:201:ARG:HB2	1.80	0.62
1:C:505:PHE:HB2	4:C:1002:GOL:H31	1.81	0.61
1:A:284:ALA:HB2	1:B:526:LEU:HD11	1.82	0.61
1:A:567:LEU:HB2	1:A:587:ILE:HD12	1.82	0.61
1:A:187:ARG:HG2	1:A:187:ARG:HH11	1.66	0.60
1:B:508:ASP:OD1	1:B:578:HIS:HE1	1.84	0.60
1:D:232:ARG:CD	1:D:394:GLY:O	2.49	0.60
1:A:441:GLN:HA	1:A:444:MET:HE2	1.84	0.60
1:B:302:GLN:H	1:B:302:GLN:NE2	1.98	0.60
1:A:202:ALA:HA	1:A:314:VAL:HG23	1.83	0.60
1:A:508:ASP:OD1	1:A:578:HIS:HE1	1.85	0.60
1:B:474:ARG:NH1	1:C:495:ASP:OD2	2.35	0.60
1:D:302:GLN:HE21	1:D:302:GLN:N	1.95	0.60
1:A:357:TRP:CD1	1:A:391:LEU:HD22	2.36	0.59
1:B:614:ASP:OD2	1:B:614:ASP:N	2.35	0.59
1:C:234:ASP:OD1	1:C:236:THR:HB	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:523:VAL:CG2	1:C:627:TYR:O	2.51	0.59
1:C:521:LEU:HG	1:C:634:THR:O	2.02	0.59
1:B:440:VAL:HG21	1:C:436:LEU:CD1	2.32	0.58
1:C:487[A]:ARG:NH1	1:C:487[A]:ARG:HG2	2.18	0.58
1:B:462:MET:HE1	1:C:494:VAL:HG11	1.86	0.58
1:D:549:HIS:HD2	1:D:550:MET:O	1.86	0.58
1:B:535:PRO:HB2	1:B:538:VAL:HG21	1.85	0.58
1:A:353:GLY:O	1:A:393:PRO:HD3	2.03	0.58
1:C:455:PRO:HA	5:C:1003:PEG:H12	1.85	0.58
1:C:433:GLU:HG3	6:C:1206:HOH:O	2.03	0.57
1:D:309:TRP:CD2	1:D:575:ARG:HD2	2.40	0.57
1:B:436:LEU:HD11	1:C:488:LEU:CD2	2.33	0.57
1:B:459:MET:HE3	4:C:1002:GOL:H12	1.85	0.57
1:B:553:ASP:HB2	1:B:602:TYR:CE1	2.41	0.56
1:A:474:ARG:NH1	1:D:495:ASP:OD2	2.39	0.56
1:B:202:ALA:HA	1:B:314:VAL:HG23	1.86	0.56
1:B:512:PRO:HD3	1:B:570:THR:HG23	1.88	0.56
1:C:195:ILE:HG21	1:C:200[A]:ARG:HG3	1.88	0.56
1:D:514:LEU:CD2	1:D:551:LEU:HD11	2.35	0.56
1:D:238:TYR:CZ	1:D:349:LEU:HB3	2.41	0.56
1:C:595:MET:HG2	1:C:622:LEU:HD11	1.88	0.56
1:A:232:ARG:HD3	1:A:394:GLY:O	2.07	0.55
1:D:431:PHE:HE2	1:D:435:ILE:HD12	1.69	0.55
6:B:1176:HOH:O	5:C:1003:PEG:H41	2.06	0.55
1:C:523:VAL:CG2	6:C:1124:HOH:O	2.55	0.55
1:D:226:GLU:OE2	1:D:361:ARG:NH1	2.40	0.55
1:B:436:LEU:HD13	1:C:436:LEU:HD22	1.88	0.55
1:A:187:ARG:NH1	6:A:1178:HOH:O	2.38	0.55
1:B:508:ASP:OD1	1:B:578:HIS:CE1	2.59	0.55
1:A:436:LEU:CD1	1:D:440:VAL:CG2	2.85	0.54
1:B:363:ARG:CG	1:B:367:GLU:OE1	2.55	0.54
1:D:417:HIS:HD2	6:D:1132:HOH:O	1.89	0.54
1:A:232:ARG:CD	1:A:394:GLY:O	2.56	0.53
1:A:542:LEU:HD22	1:A:638:LEU:HD11	1.90	0.53
1:C:456:ARG:HE	5:C:1003:PEG:C4	2.21	0.53
1:A:379:GLN:OE1	1:A:406:GLN:NE2	2.39	0.53
1:D:287:TRP:CE3	1:D:287:TRP:HA	2.44	0.53
1:A:526:LEU:HD12	1:A:527:PRO:HD2	1.91	0.53
1:C:287:TRP:HA	1:C:287:TRP:CE3	2.43	0.53
1:C:487[A]:ARG:CG	1:C:487[A]:ARG:NH1	2.58	0.53
1:A:569:TYR:OH	1:A:629:LYS:HE3	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:310:GLN:O	1:B:314:VAL:HG13	2.07	0.53
1:C:232:ARG:CD	1:C:394:GLY:O	2.54	0.53
1:C:266:ARG:NH1	1:C:292:ALA:O	2.41	0.52
1:C:538:VAL:HG21	1:D:291:GLN:HG3	1.90	0.52
1:B:514:LEU:CD2	1:B:551:LEU:HD11	2.38	0.52
1:D:315:LEU:HD23	1:D:420:LEU:HD11	1.90	0.52
1:B:297:ARG:HE	1:B:299:LEU:CD2	2.21	0.52
1:B:512:PRO:HD3	1:B:570:THR:CG2	2.39	0.52
1:C:310:GLN:O	1:C:314:VAL:HG13	2.10	0.52
1:D:540:ALA:HB1	1:D:638:LEU:HB3	1.91	0.52
1:D:349:LEU:HD22	1:D:396:LEU:HD12	1.92	0.51
1:A:588:TYR:HB3	1:A:590:GLN:HE22	1.75	0.51
1:C:487[A]:ARG:HH11	1:C:487[A]:ARG:CA	2.23	0.51
1:A:436:LEU:HD12	1:D:440:VAL:HG21	1.92	0.51
1:A:553:ASP:HB2	1:A:602:TYR:CE1	2.46	0.51
1:B:485:VAL:HG22	1:C:436:LEU:HD21	1.92	0.51
1:D:363:ARG:HG2	1:D:367:GLU:OE1	2.10	0.51
1:D:514:LEU:HD22	1:D:551:LEU:HD11	1.91	0.51
1:A:521:LEU:HG	1:A:634:THR:O	2.10	0.51
1:A:485:VAL:O	1:A:488:LEU:HB2	2.11	0.51
1:B:417:HIS:HD2	6:B:1106:HOH:O	1.94	0.51
1:D:608:VAL:O	1:D:611:LEU:HB2	2.11	0.51
1:A:436:LEU:HD13	1:D:440:VAL:CG2	2.41	0.50
1:B:549:HIS:CE1	1:B:633:LEU:HD11	2.46	0.50
1:C:523:VAL:HG22	1:C:627:TYR:O	2.12	0.50
1:D:487[B]:ARG:HG3	1:D:487[B]:ARG:HH11	1.77	0.50
1:B:254:GLU:HG2	1:B:304:PHE:CE1	2.46	0.50
1:B:514:LEU:HD21	1:B:551:LEU:HD11	1.94	0.50
1:C:542:LEU:HD22	1:C:546:THR:HG21	1.94	0.50
1:A:590:GLN:H	1:A:590:GLN:HE21	1.56	0.50
1:B:302:GLN:HE21	1:B:302:GLN:N	2.03	0.50
1:D:615:SER:HB2	1:D:618:ASP:H	1.76	0.50
1:A:534:GLU:CG	1:A:535:PRO:HD2	2.42	0.50
1:A:297:ARG:NH2	1:A:299:LEU:HD21	2.26	0.49
1:C:284:ALA:O	1:C:288:SER:HB3	2.13	0.49
1:C:363:ARG:HG2	1:C:367:GLU:OE1	2.12	0.49
1:B:427:THR:HG22	1:B:430:ASP:N	2.24	0.49
1:B:433[A]:GLU:HG3	6:C:1204:HOH:O	2.11	0.49
1:D:487[B]:ARG:HG3	1:D:487[B]:ARG:NH1	2.28	0.49
1:D:553:ASP:HB2	1:D:602:TYR:CE1	2.47	0.49
1:B:523:VAL:HG22	6:B:1135:HOH:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:435:ILE:HD13	1:C:492:ALA:HB1	1.93	0.49
1:C:290:TYR:CD1	1:C:329:LEU:HD13	2.48	0.49
1:A:310:GLN:HA	1:A:513:VAL:HG21	1.94	0.48
1:C:456:ARG:HE	5:C:1003:PEG:C3	2.26	0.48
1:A:549:HIS:HD2	1:A:550:MET:O	1.96	0.48
1:B:231:ARG:NH2	1:B:389:THR:OG1	2.47	0.48
1:B:431:PHE:CE2	1:B:435:ILE:HD12	2.49	0.48
1:C:302:GLN:H	1:C:302:GLN:NE2	2.06	0.48
1:A:508:ASP:OD1	1:A:578:HIS:CE1	2.65	0.48
1:C:456:ARG:HE	5:C:1003:PEG:H32	1.79	0.48
1:A:542:LEU:HD13	1:A:546:THR:HG21	1.96	0.48
1:A:301:PRO:HG2	1:A:325:SER:OG	2.14	0.48
1:C:362:PRO:HA	6:C:1155:HOH:O	2.12	0.48
1:A:427:THR:HG22	1:A:430:ASP:N	2.23	0.47
1:B:435:ILE:HD11	1:B:494:VAL:CA	2.37	0.47
1:B:567:LEU:HB2	1:B:587:ILE:HD13	1.96	0.47
1:D:575:ARG:HG3	6:D:1147:HOH:O	2.15	0.47
1:C:325:SER:HA	1:C:419:THR:O	2.14	0.47
1:C:517:ARG:HG2	1:C:521:LEU:HD22	1.97	0.47
1:C:633:LEU:C	1:C:633:LEU:HD12	2.35	0.47
1:D:570:THR:CG2	6:D:1128:HOH:O	2.54	0.47
1:A:517[A]:ARG:HG2	1:A:521:LEU:HD22	1.96	0.47
1:B:611:LEU:O	1:B:613:CYS:N	2.48	0.47
1:C:205:LEU:HD23	1:C:314:VAL:HG22	1.97	0.47
1:D:431:PHE:HE2	1:D:435:ILE:CD1	2.27	0.47
1:B:435:ILE:HG13	1:B:497:VAL:HG21	1.97	0.47
1:D:205:LEU:HD23	1:D:314:VAL:HG22	1.97	0.47
1:D:567:LEU:HB2	1:D:587:ILE:HD12	1.97	0.47
1:B:495:ASP:CG	1:C:474:ARG:HH22	2.18	0.47
1:A:608:VAL:HA	1:A:611:LEU:HD22	1.97	0.46
1:C:232:ARG:HD3	1:C:237:TYR:CD1	2.51	0.46
1:C:284:ALA:HA	1:D:528:ILE:HD12	1.97	0.46
1:A:534:GLU:HG3	1:A:535:PRO:HD2	1.97	0.46
1:D:353:GLY:O	1:D:393:PRO:HD3	2.16	0.46
1:A:310:GLN:O	1:A:314:VAL:HG13	2.16	0.46
1:A:238:TYR:CZ	1:A:349:LEU:HB3	2.51	0.46
1:B:232:ARG:CD	1:B:394:GLY:O	2.64	0.46
1:D:242:PHE:CE2	1:D:327:VAL:HG11	2.51	0.46
1:C:587:ILE:CD1	1:C:595:MET:HG3	2.38	0.46
1:D:252:ARG:HG3	1:D:253:ASN:ND2	2.31	0.46
1:A:187:ARG:HH11	1:A:187:ARG:CG	2.28	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:325:SER:HA	1:A:419:THR:O	2.16	0.46
1:A:633:LEU:C	1:A:633:LEU:HD12	2.36	0.45
1:B:495:ASP:OD1	1:C:474:ARG:NH2	2.48	0.45
1:A:436:LEU:CD1	1:D:440:VAL:HG21	2.46	0.45
1:A:275:LEU:O	1:A:277:PRO:HD3	2.17	0.45
1:D:436:LEU:O	1:D:440:VAL:HG23	2.16	0.45
1:B:456:ARG:HD3	1:C:219:TYR:CE1	2.51	0.45
1:A:287:TRP:HA	1:A:287:TRP:CE3	2.52	0.45
1:C:487[A]:ARG:HH11	1:C:487[A]:ARG:HG2	1.70	0.45
1:A:555:ILE:O	1:A:569:TYR:HA	2.17	0.45
1:B:549:HIS:HD2	1:B:550:MET:O	2.00	0.45
1:D:362:PRO:HD3	1:D:403:PHE:CE2	2.52	0.45
1:B:325:SER:HA	1:B:419:THR:O	2.17	0.45
1:A:567:LEU:HB2	1:A:587:ILE:HD11	1.98	0.44
1:D:335:GLN:HG3	1:D:407:ALA:O	2.17	0.44
1:A:194:ARG:CG	1:A:194:ARG:HH11	2.30	0.44
1:A:244:THR:HG21	1:B:530:TRP:CE2	2.53	0.44
1:D:613:CYS:HB2	1:D:619:GLN:HG3	2.00	0.44
1:B:219:TYR:HB3	5:C:1003:PEG:C4	2.48	0.44
1:C:435:ILE:HD11	1:C:494:VAL:HA	2.00	0.44
1:D:202:ALA:HA	1:D:314:VAL:HG23	2.00	0.44
1:D:363:ARG:HD3	1:D:404:ILE:CD1	2.48	0.44
1:B:310:GLN:HA	1:B:513:VAL:HG21	1.99	0.44
1:C:271:ARG:CG	1:C:272:ARG:H	2.04	0.44
1:B:232:ARG:HD2	1:B:394:GLY:O	2.18	0.44
1:B:503:LYS:HD2	1:B:568:TYR:CZ	2.52	0.44
1:B:585:LEU:HD12	1:B:585:LEU:C	2.39	0.43
1:B:254:GLU:CG	1:B:304:PHE:CE1	3.02	0.43
1:D:325:SER:HA	1:D:419:THR:O	2.19	0.43
1:B:363:ARG:HG2	1:B:363:ARG:H	1.71	0.43
1:C:322:MET:O	1:C:422:THR:HG22	2.18	0.43
1:D:301:PRO:HG2	1:D:325:SER:OG	2.18	0.43
1:C:427:THR:CG2	1:C:429:GLY:H	2.32	0.43
1:B:205:LEU:HD23	1:B:315:LEU:HD13	2.01	0.43
1:D:226:GLU:HG3	6:D:1180:HOH:O	2.19	0.43
1:B:485:VAL:O	1:B:488:LEU:HB2	2.19	0.43
1:D:310:GLN:O	1:D:314:VAL:HG13	2.19	0.43
1:A:234:ASP:OD1	1:A:236:THR:HB	2.18	0.42
1:A:495:ASP:OD2	1:D:474:ARG:NH2	2.33	0.42
1:B:341:TYR:CZ	1:B:374:SER:HB3	2.54	0.42
1:C:556:ALA:HA	1:C:568:TYR:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:363:ARG:HG2	1:A:367:GLU:OE1	2.19	0.42
1:B:254:GLU:CG	1:B:304:PHE:CD1	2.94	0.42
1:A:252:ARG:HG3	1:A:253:ASN:ND2	2.34	0.42
1:B:312:LEU:HB3	1:B:510:LEU:CD1	2.49	0.42
1:B:349:LEU:HD22	1:B:396:LEU:HD12	2.02	0.42
1:C:185:LEU:HD22	1:C:241:LEU:HB2	2.00	0.42
1:C:210:ILE:O	1:C:213:MET:HB3	2.18	0.42
1:C:216[B]:ASP:OD1	1:C:217:HIS:N	2.50	0.42
1:C:528:ILE:HD12	1:D:284:ALA:HA	2.01	0.42
1:D:192:LEU:HG	1:D:201:ARG:HB2	2.01	0.42
1:B:427:THR:HG23	1:C:450:PHE:O	2.18	0.42
1:C:210:ILE:HD12	1:C:213:MET:HG3	2.00	0.42
1:C:587:ILE:HD13	1:C:595:MET:CG	2.42	0.42
1:A:322:MET:O	1:A:422:THR:CG2	2.68	0.42
1:B:392:GLU:O	1:B:393:PRO:C	2.57	0.42
1:C:220:ARG:HE	1:C:220:ARG:HB2	1.59	0.41
1:C:526:LEU:HA	1:C:527:PRO:HD3	1.87	0.41
1:B:399:PHE:HA	1:B:400:PRO:HD3	1.90	0.41
1:B:503:LYS:NZ	6:B:1173:HOH:O	2.53	0.41
1:B:546:THR:O	1:B:608:VAL:HG23	2.20	0.41
1:D:466:HIS:HE1	6:D:1193:HOH:O	2.03	0.41
1:A:507:HIS:HE1	1:A:580:GLU:O	2.02	0.41
1:D:514:LEU:HD21	1:D:551:LEU:HD11	2.02	0.41
1:A:235:HIS:HA	1:A:393:PRO:O	2.21	0.41
1:D:512:PRO:HD3	1:D:570:THR:CG2	2.51	0.41
1:A:441:GLN:HA	1:A:444:MET:CE	2.48	0.41
1:B:369:LEU:HA	1:B:401:ARG:HG3	2.03	0.41
1:B:555:ILE:HG22	1:B:570:THR:HG21	2.03	0.41
1:A:427:THR:HG23	1:D:450:PHE:O	2.20	0.41
1:C:185:LEU:CD2	1:C:241:LEU:HB2	2.50	0.41
1:C:487[A]:ARG:HB3	1:C:487[A]:ARG:NH1	2.34	0.41
1:D:266:ARG:NH1	1:D:292:ALA:O	2.54	0.41
1:D:345:GLU:OE1	1:D:400:PRO:HA	2.20	0.41
1:B:436:LEU:CD1	1:C:436:LEU:HD22	2.49	0.40
1:B:544:THR:O	1:B:607[A]:ARG:HG2	2.21	0.40
1:C:209:LEU:HD13	1:C:311:PHE:HZ	1.85	0.40
1:C:341:TYR:CZ	1:C:374:SER:HB3	2.57	0.40
1:C:588:TYR:HB3	1:C:590:GLN:HE22	1.87	0.40
1:D:485:VAL:O	1:D:488:LEU:HB2	2.21	0.40
1:D:186:ARG:NH1	1:D:239[A]:GLN:OE1	2.55	0.40
1:D:553:ASP:HB2	1:D:602:TYR:CD1	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:310:GLN:HA	1:C:513:VAL:HG21	2.04	0.40
1:C:427:THR:HG22	1:C:429:GLY:N	2.37	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	458/463 (99%)	447 (98%)	11 (2%)	0	100	100
1	B	470/463 (102%)	459 (98%)	11 (2%)	0	100	100
1	C	458/463 (99%)	447 (98%)	11 (2%)	0	100	100
1	D	462/463 (100%)	447 (97%)	15 (3%)	0	100	100
All	All	1848/1852 (100%)	1800 (97%)	48 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	396/395 (100%)	348 (88%)	48 (12%)	5	4
1	B	405/395 (102%)	357 (88%)	48 (12%)	5	5
1	C	396/395 (100%)	344 (87%)	52 (13%)	4	3

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	D	398/395 (101%)	352 (88%)	46 (12%)	5 5
All	All	1595/1580 (101%)	1401 (88%)	194 (12%)	5 4

All (194) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	187	ARG
1	A	189	LEU
1	A	194	ARG
1	A	209	LEU
1	A	231	ARG
1	A	232	ARG
1	A	233	GLN
1	A	236	THR
1	A	239	GLN
1	A	251	LEU
1	A	257	GLN
1	A	263	ASP
1	A	272	ARG
1	A	289	LEU
1	A	302	GLN
1	A	312	LEU
1	A	315	LEU
1	A	318	GLN
1	A	329	LEU
1	A	348	VAL
1	A	349	LEU
1	A	355	LYS
1	A	359	VAL
1	A	361	ARG
1	A	363	ARG
1	A	366[A]	THR
1	A	366[B]	THR
1	A	391	LEU
1	A	422	THR
1	A	427	THR
1	A	432	LEU
1	A	435	ILE
1	A	454	LEU
1	A	468	ASP
1	A	478	MET
1	A	479	GLU

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Mol	Chain	Res	Type
1	A	488	LEU
1	A	521	LEU
1	A	542	LEU
1	A	551	LEU
1	A	558	LEU
1	A	579	LEU
1	A	590	GLN
1	A	591	GLN
1	A	595	MET
1	A	607	ARG
1	A	611	LEU
1	A	622	LEU
1	B	182	SER
1	B	186	ARG
1	B	189	LEU
1	B	209	LEU
1	B	229	LEU
1	B	232	ARG
1	B	251	LEU
1	B	252	ARG
1	B	255	GLU
1	B	257	GLN
1	B	272	ARG
1	B	295	SER
1	B	302	GLN
1	B	312	LEU
1	B	315	LEU
1	B	318	GLN
1	B	329	LEU
1	B	348	VAL
1	B	349	LEU
1	B	359	VAL
1	B	361	ARG
1	B	363	ARG
1	B	366[A]	THR
1	B	366[B]	THR
1	B	379[A]	GLN
1	B	379[B]	GLN
1	B	391	LEU
1	B	409	CYS
1	B	420	LEU
1	B	422	THR

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Mol	Chain	Res	Type
1	B	427	THR
1	B	432	LEU
1	B	433[A]	GLU
1	B	433[B]	GLU
1	B	435	ILE
1	B	436	LEU
1	B	454	LEU
1	B	479	GLU
1	B	488	LEU
1	B	523	VAL
1	B	526	LEU
1	B	558	LEU
1	B	570	THR
1	B	575	ARG
1	B	578	HIS
1	B	579	LEU
1	B	595	MET
1	B	614	ASP
1	C	189	LEU
1	C	192	LEU
1	C	201	ARG
1	C	221[A]	ARG
1	C	221[B]	ARG
1	C	226	GLU
1	C	229	LEU
1	C	232	ARG
1	C	249	SER
1	C	251	LEU
1	C	274	THR
1	C	288	SER
1	C	289	LEU
1	C	302	GLN
1	C	306	THR
1	C	307	THR
1	C	312	LEU
1	C	315	LEU
1	C	329	LEU
1	C	348	VAL
1	C	349	LEU
1	C	359	VAL
1	C	363	ARG
1	C	366	THR

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Mol	Chain	Res	Type
1	C	384	GLU
1	C	387	LEU
1	C	420	LEU
1	C	422	THR
1	C	427	THR
1	C	435	ILE
1	C	470	LYS
1	C	487[A]	ARG
1	C	487[B]	ARG
1	C	517	ARG
1	C	521	LEU
1	C	523	VAL
1	C	528	ILE
1	C	529	ARG
1	C	551	LEU
1	C	558	LEU
1	C	570	THR
1	C	578	HIS
1	C	579	LEU
1	C	581	GLU
1	C	591	GLN
1	C	593	ASP
1	C	595	MET
1	C	606	VAL
1	C	607[A]	ARG
1	C	607[B]	ARG
1	C	611	LEU
1	C	622	LEU
1	D	189	LEU
1	D	209	LEU
1	D	221	ARG
1	D	226	GLU
1	D	229	LEU
1	D	232	ARG
1	D	235	HIS
1	D	251	LEU
1	D	255	GLU
1	D	257	GLN
1	D	288	SER
1	D	302	GLN
1	D	312	LEU
1	D	315	LEU

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Mol	Chain	Res	Type
1	D	329	LEU
1	D	349	LEU
1	D	354	ARG
1	D	359	VAL
1	D	361	ARG
1	D	363	ARG
1	D	380	ASP
1	D	384[A]	GLU
1	D	384[B]	GLU
1	D	391	LEU
1	D	410	GLN
1	D	422	THR
1	D	427	THR
1	D	432	LEU
1	D	435	ILE
1	D	454	LEU
1	D	478	MET
1	D	479	GLU
1	D	488	LEU
1	D	521	LEU
1	D	526	LEU
1	D	538	VAL
1	D	561	GLU
1	D	570	THR
1	D	578	HIS
1	D	579	LEU
1	D	587	ILE
1	D	590	GLN
1	D	595	MET
1	D	606	VAL
1	D	611	LEU
1	D	622	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	253	ASN
1	A	302	GLN
1	A	379	GLN
1	A	406	GLN
1	A	441	GLN
1	A	507	HIS

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Mol	Chain	Res	Type
1	A	549	HIS
1	A	578	HIS
1	A	590	GLN
1	B	253	ASN
1	B	257	GLN
1	B	302	GLN
1	B	326	ASN
1	B	410	GLN
1	B	417	HIS
1	B	507	HIS
1	B	549	HIS
1	B	578	HIS
1	B	590	GLN
1	C	253	ASN
1	C	302	GLN
1	C	318	GLN
1	C	326	ASN
1	C	441	GLN
1	C	507	HIS
1	C	549	HIS
1	C	578	HIS
1	C	590	GLN
1	D	253	ASN
1	D	302	GLN
1	D	318	GLN
1	D	417	HIS
1	D	441	GLN
1	D	507	HIS
1	D	549	HIS
1	D	578	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 7 ligands modelled in this entry, 4 are monoatomic - leaving 3 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	ACT	A	1002	-	3,3,3	0.78	0	3,3,3	1.47	0
4	GOL	C	1002	-	5,5,5	0.56	0	5,5,5	0.80	0
5	PEG	C	1003	-	6,6,6	0.70	0	5,5,5	0.69	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
4	GOL	C	1002	-	-	4/4/4/4	-
5	PEG	C	1003	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	1002	GOL	O1-C1-C2-C3
4	C	1002	GOL	C1-C2-C3-O3
5	C	1003	PEG	C1-C2-O2-C3
5	C	1003	PEG	O2-C3-C4-O4
4	C	1002	GOL	O2-C2-C3-O3
4	C	1002	GOL	O1-C1-C2-O2

There are no ring outliers.

2 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	1002	GOL	3	0
5	C	1003	PEG	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 (i)

6.1 Protein, DNA and RNA chains (i)

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, 95th 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	455/463 (98%)	-0.12	5 (1%)	80	84	24, 38, 57, 75	23 (5%)
1	B	458/463 (98%)	-0.15	10 (2%)	62	68	22, 37, 66, 77	31 (6%)
1	C	455/463 (98%)	-0.35	2 (0%)	92	94	23, 36, 59, 73	26 (5%)
1	D	457/463 (98%)	-0.02	14 (3%)	49	54	26, 41, 65, 75	29 (6%)
All	All	1825/1852 (98%)	-0.16	31 (1%)	70	75	22, 38, 62, 77	109 (5%)

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	539	GLY	9.4
1	D	268	ILE	6.1
1	B	538	VAL	4.6
1	D	269	ASN	4.5
1	B	539	GLY	4.4
1	B	267	TYR	3.9
1	C	538	VAL	3.9
1	B	268	ILE	3.6
1	B	562	GLY	3.4
1	D	267	TYR	3.2
1	A	271	ARG	3.1
1	C	267	TYR	3.0
1	D	182	SER	2.8
1	A	411	ASP	2.8
1	D	271	ARG	2.8
1	D	636	MET	2.7
1	A	337	PHE	2.7
1	D	300[A]	CYS	2.7
1	D	470	LYS	2.6
1	B	269	ASN	2.6
1	D	336	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	409	CYS	2.4
1	D	413	VAL	2.4
1	B	271	ARG	2.3
1	D	538	VAL	2.3
1	B	181	GLY	2.3
1	D	576	VAL	2.3
1	B	531	GLU	2.1
1	A	413	VAL	2.0
1	D	411	ASP	2.0
1	B	270	GLY	2.0

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 monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	PEG	C	1003	7/7	0.70	0.26	46,47,53,54	4
3	ACT	A	1002	4/4	0.86	0.12	58,59,59,59	0
4	GOL	C	1002	6/6	0.91	0.17	37,43,45,47	0
2	FE	D	1001	1/1	0.92	0.06	80,80,80,80	0
2	FE	B	1001	1/1	0.97	0.03	59,59,59,59	0
2	FE	A	1001	1/1	0.98	0.09	48,48,48,48	0
2	FE	C	1001	1/1	0.98	0.07	48,48,48,48	0

6.5 Other polymers (i)

There are no such residues in this entry.