



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 02:47 PM UTC

PDB ID : 4O6O / pdb_00004o6o
Title : Structural and functional studies the characterization of Cys4 Zinc-finger motif
in the recombination mediator protein RecR
Authors : Tang, Q.; Liu, Y.P.; Yan, X.X.; Liang, D.C.
Deposited on : 2013-12-23
Resolution : 3.00 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 ⓘ 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 ⓘ](#)) were used in the production of this report:

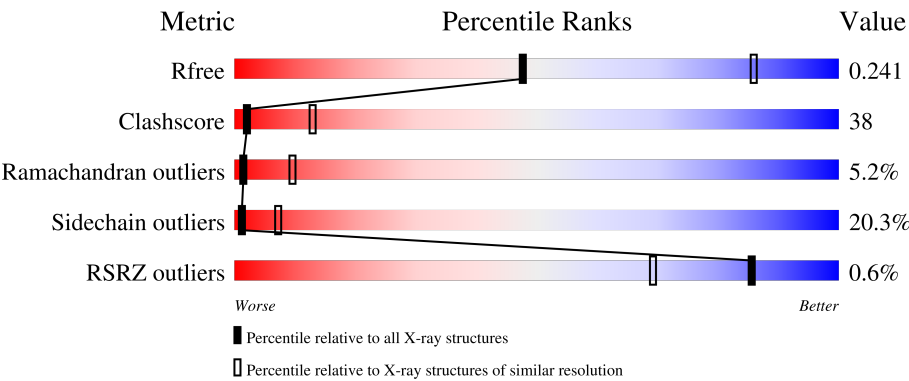
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

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 3.00 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}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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 $\leq 5\%$. 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	212	41%41%10%•7%
1	B	212	35%38%18%•7%
1	C	212	32%41%18%•7%
1	D	212	% 40%40%12%•6%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6209 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 Recombination protein RecR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	197	Total	C	N	O	S	0	0	0
			1518	968	259	283	8			
1	B	197	Total	C	N	O	S	0	0	0
			1502	954	255	285	8			
1	C	197	Total	C	N	O	S	0	0	0
			1518	966	257	287	8			
1	D	199	Total	C	N	O	S	0	0	0
			1520	968	260	283	9			

There are 56 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-15	GLY	-	expression tag	UNP Q8RDI4
A	-14	SER	-	expression tag	UNP Q8RDI4
A	-13	SER	-	expression tag	UNP Q8RDI4
A	-12	HIS	-	expression tag	UNP Q8RDI4
A	-11	HIS	-	expression tag	UNP Q8RDI4
A	-10	HIS	-	expression tag	UNP Q8RDI4
A	-9	HIS	-	expression tag	UNP Q8RDI4
A	-8	HIS	-	expression tag	UNP Q8RDI4
A	-7	HIS	-	expression tag	UNP Q8RDI4
A	-6	SER	-	expression tag	UNP Q8RDI4
A	-5	GLN	-	expression tag	UNP Q8RDI4
A	-4	ASP	-	expression tag	UNP Q8RDI4
A	-3	PRO	-	expression tag	UNP Q8RDI4
A	55	GLY	CYS	engineered mutation	UNP Q8RDI4
B	-15	GLY	-	expression tag	UNP Q8RDI4
B	-14	SER	-	expression tag	UNP Q8RDI4
B	-13	SER	-	expression tag	UNP Q8RDI4
B	-12	HIS	-	expression tag	UNP Q8RDI4
B	-11	HIS	-	expression tag	UNP Q8RDI4
B	-10	HIS	-	expression tag	UNP Q8RDI4
B	-9	HIS	-	expression tag	UNP Q8RDI4

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-8	HIS	-	expression tag	UNP Q8RDI4
B	-7	HIS	-	expression tag	UNP Q8RDI4
B	-6	SER	-	expression tag	UNP Q8RDI4
B	-5	GLN	-	expression tag	UNP Q8RDI4
B	-4	ASP	-	expression tag	UNP Q8RDI4
B	-3	PRO	-	expression tag	UNP Q8RDI4
B	55	GLY	CYS	engineered mutation	UNP Q8RDI4
C	-15	GLY	-	expression tag	UNP Q8RDI4
C	-14	SER	-	expression tag	UNP Q8RDI4
C	-13	SER	-	expression tag	UNP Q8RDI4
C	-12	HIS	-	expression tag	UNP Q8RDI4
C	-11	HIS	-	expression tag	UNP Q8RDI4
C	-10	HIS	-	expression tag	UNP Q8RDI4
C	-9	HIS	-	expression tag	UNP Q8RDI4
C	-8	HIS	-	expression tag	UNP Q8RDI4
C	-7	HIS	-	expression tag	UNP Q8RDI4
C	-6	SER	-	expression tag	UNP Q8RDI4
C	-5	GLN	-	expression tag	UNP Q8RDI4
C	-4	ASP	-	expression tag	UNP Q8RDI4
C	-3	PRO	-	expression tag	UNP Q8RDI4
C	55	GLY	CYS	engineered mutation	UNP Q8RDI4
D	-15	GLY	-	expression tag	UNP Q8RDI4
D	-14	SER	-	expression tag	UNP Q8RDI4
D	-13	SER	-	expression tag	UNP Q8RDI4
D	-12	HIS	-	expression tag	UNP Q8RDI4
D	-11	HIS	-	expression tag	UNP Q8RDI4
D	-10	HIS	-	expression tag	UNP Q8RDI4
D	-9	HIS	-	expression tag	UNP Q8RDI4
D	-8	HIS	-	expression tag	UNP Q8RDI4
D	-7	HIS	-	expression tag	UNP Q8RDI4
D	-6	SER	-	expression tag	UNP Q8RDI4
D	-5	GLN	-	expression tag	UNP Q8RDI4
D	-4	ASP	-	expression tag	UNP Q8RDI4
D	-3	PRO	-	expression tag	UNP Q8RDI4
D	55	GLY	CYS	engineered mutation	UNP Q8RDI4

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

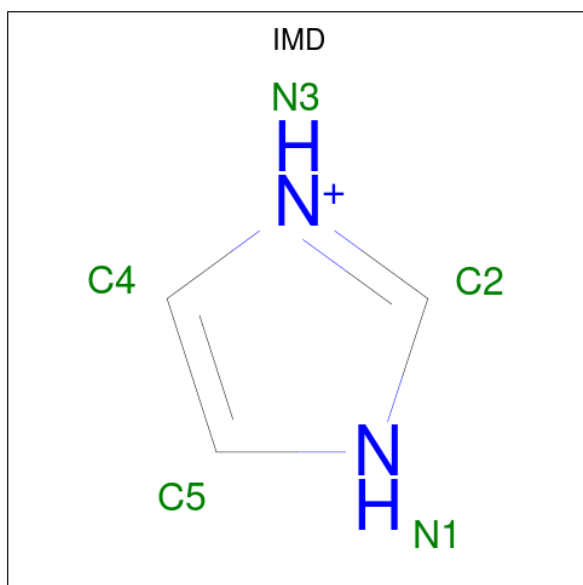
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Zn 1 1	0	0
2	B	1	Total Zn 1 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	C	1	Total	Zn	0	0
			1	1		
2	D	1	Total	Zn	0	0
			1	1		

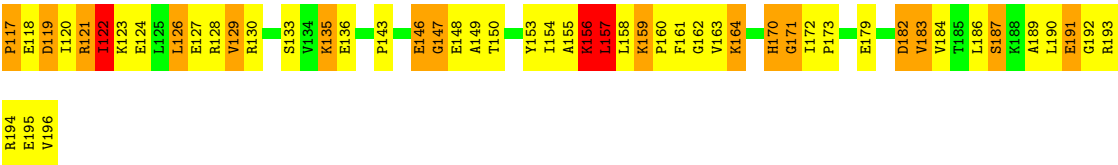
- Molecule 3 is IMIDAZOLE (CCD ID: IMD) (formula: $C_3H_5N_2$).



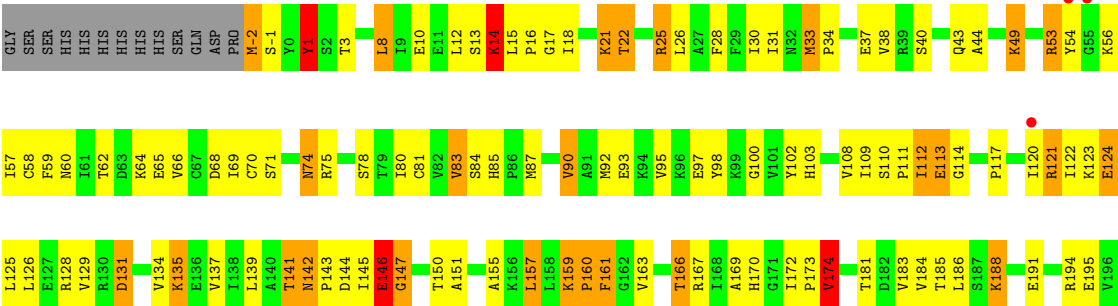
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	N	0	0
			5	3	2		
3	A	1	Total	C	N	0	0
			5	3	2		
3	B	1	Total	C	N	0	0
			5	3	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	28	Total	O	0	0
			28	28		
4	B	39	Total	O	0	0
			39	39		
4	C	26	Total	O	0	0
			26	26		
4	D	39	Total	O	0	0
			39	39		



• Molecule 1: Recombination protein RecR



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	90.60Å 67.91Å 94.36Å 90.00° 92.98° 90.00°	Depositor
Resolution (Å)	20.00 – 3.00 20.00 – 3.00	Depositor EDS
% Data completeness (in resolution range)	98.5 (20.00-3.00) 98.1 (20.00-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.37 (at 2.98Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.220 , 0.255 0.227 , 0.241	Depositor DCC
R_{free} test set	1151 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	61.3	Xtriage
Anisotropy	0.728	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.24 , 54.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.000 for l,k,-h 0.000 for h,-k,-l 0.000 for l,-k,h	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6209	wwPDB-VP
Average B, all atoms (Å ²)	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 52.72 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.6717e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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: IMD, ZN

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	1.04	0/1542	1.22	6/2083 (0.3%)
1	B	1.01	0/1524	1.36	16/2060 (0.8%)
1	C	1.00	0/1542	1.34	15/2085 (0.7%)
1	D	1.04	0/1543	1.38	16/2085 (0.8%)
All	All	1.02	0/6151	1.32	53/8313 (0.6%)

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	B	0	1
1	C	0	1
All	All	0	2

There are no bond length outliers.

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	113	GLU	CB-CA-C	-16.10	88.29	111.80
1	B	1	TYR	N-CA-C	12.06	125.02	110.91
1	C	116	GLY	CA-C-N	11.31	133.97	119.84
1	C	116	GLY	C-N-CA	11.31	133.97	119.84
1	C	163	VAL	N-CA-C	11.05	120.35	111.62
1	B	2	SER	CB-CA-C	-10.17	88.02	110.19
1	B	0	TYR	CB-CA-C	-9.86	91.36	110.10
1	D	14	LYS	N-CA-C	-9.62	101.54	113.38
1	D	112	ILE	N-CA-CB	9.59	122.49	109.84
1	C	122	ILE	CB-CA-C	-8.91	102.97	111.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	28	PHE	N-CA-C	8.51	120.17	111.07
1	B	0	TYR	CA-C-N	7.54	134.32	122.93
1	B	0	TYR	C-N-CA	7.54	134.32	122.93
1	A	85	HIS	CA-C-N	7.39	128.04	119.47
1	A	85	HIS	C-N-CA	7.39	128.04	119.47
1	B	109	ILE	N-CA-C	7.29	114.00	106.21
1	D	33	MET	CA-C-N	7.22	128.35	119.98
1	D	33	MET	C-N-CA	7.22	128.35	119.98
1	D	170	HIS	CA-C-N	-6.91	116.84	122.16
1	D	170	HIS	C-N-CA	-6.91	116.84	122.16
1	C	163	VAL	N-CA-CB	-6.79	106.07	111.64
1	B	0	TYR	N-CA-C	-6.74	92.13	111.00
1	B	14	LYS	N-CA-C	-6.62	105.49	113.97
1	C	119	ASP	N-CA-C	-6.61	105.18	113.18
1	B	2	SER	N-CA-C	-6.57	102.33	110.41
1	B	145	ILE	N-CA-C	-6.54	103.41	113.16
1	B	23	ALA	N-CA-C	-6.44	104.68	112.54
1	D	114	GLY	N-CA-C	6.41	128.37	113.18
1	D	142	ASN	N-CA-C	6.37	116.93	109.60
1	C	171	GLY	CA-C-N	-6.20	116.57	123.02
1	C	171	GLY	C-N-CA	-6.20	116.57	123.02
1	C	187	SER	N-CA-C	-6.09	103.96	111.33
1	A	33	MET	CA-C-N	6.06	126.08	119.89
1	A	33	MET	C-N-CA	6.06	126.08	119.89
1	B	154	ILE	N-CA-C	-6.05	103.72	110.62
1	C	182	ASP	N-CA-C	6.02	118.33	109.24
1	D	80	ILE	N-CA-C	5.89	116.33	107.80
1	D	112	ILE	N-CA-C	-5.83	100.58	107.70
1	D	142	ASN	CA-C-N	5.56	126.79	119.84
1	D	142	ASN	C-N-CA	5.56	126.79	119.84
1	D	1	TYR	N-CA-C	5.54	116.39	108.74
1	C	115	VAL	N-CA-C	5.53	117.86	109.12
1	B	1	TYR	CB-CA-C	-5.42	102.79	112.27
1	C	70	CYS	N-CA-C	-5.41	106.52	113.01
1	A	4	SER	N-CA-C	-5.38	105.41	111.28
1	B	92	MET	N-CA-C	5.32	117.77	111.33
1	A	60	ASN	N-CA-C	-5.30	103.89	110.41
1	C	71	SER	N-CA-C	-5.25	107.41	112.97
1	D	8	LEU	N-CA-C	5.23	117.39	111.11
1	C	3	THR	N-CA-C	5.20	117.35	111.11
1	C	170	HIS	N-CA-C	-5.10	101.38	109.59
1	B	136	GLU	N-CA-C	5.07	117.32	108.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	81	CYS	N-CA-C	5.04	117.33	108.56

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	0	TYR	Peptide
1	C	162	GLY	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	1518	0	1569	121	0
1	B	1502	0	1540	129	0
1	C	1518	0	1555	147	0
1	D	1520	0	1560	131	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	10	0	0
3	B	5	0	5	1	0
4	A	28	0	0	8	0
4	B	39	0	0	9	0
4	C	26	0	0	9	0
4	D	39	0	0	15	0
All	All	6209	0	6239	467	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 38.

All (467) 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:146:GLU:HG2	4:B:314:HOH:O	1.31	1.25

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:124:GLU:O	1:A:128:ARG:HG3	1.45	1.17
1:D:15:LEU:HB2	1:D:18:ILE:HG13	1.29	1.10
1:C:30:ILE:HA	1:C:33:MET:HE2	1.36	1.08
1:D:13:SER:HA	1:D:18:ILE:HG21	1.28	1.08
1:D:13:SER:HA	1:D:18:ILE:CG2	1.84	1.07
1:D:25:ARG:HG3	1:D:25:ARG:HH11	1.20	1.03
1:A:168:ILE:HD11	1:B:190:LEU:HA	1.38	1.03
1:A:195:GLU:O	1:A:196:VAL:HG22	1.59	1.00
1:D:121:ARG:HH11	1:D:121:ARG:HG3	1.25	0.97
1:C:83:VAL:HG13	1:C:84:SER:H	1.29	0.97
1:A:12:LEU:C	1:A:18:ILE:HD11	1.90	0.96
1:B:109:ILE:HG13	1:B:109:ILE:O	1.62	0.96
1:A:122:ILE:HG23	1:A:123:LYS:HD3	1.45	0.94
1:C:191:GLU:HB2	4:D:312:HOH:O	1.69	0.90
1:C:126:LEU:HB2	4:C:321:HOH:O	1.71	0.89
1:D:103:HIS:HB2	1:D:128:ARG:NH1	1.89	0.88
1:B:109:ILE:HD11	1:B:149:ALA:HB1	1.54	0.88
1:C:30:ILE:HA	1:C:33:MET:CE	2.03	0.87
1:B:94:LYS:O	1:B:96:LYS:HD2	1.75	0.84
1:A:142:ASN:ND2	1:B:177:ASP:HB2	1.91	0.84
1:A:180:TYR:OH	1:C:21:LYS:HD2	1.76	0.83
1:B:76:ASP:OD2	1:B:79:THR:HG23	1.77	0.83
1:C:14:LYS:HB3	4:C:306:HOH:O	1.76	0.83
1:C:190:LEU:O	1:C:193:ARG:HG2	1.79	0.83
1:A:18:ILE:HG13	1:A:18:ILE:O	1.78	0.82
1:A:168:ILE:CD1	1:B:190:LEU:HA	2.11	0.81
1:B:21:LYS:HG3	1:B:22:THR:H	1.45	0.80
1:D:25:ARG:HG3	1:D:25:ARG:NH1	1.94	0.80
1:D:30:ILE:O	1:D:33:MET:HB2	1.83	0.78
1:C:171:GLY:HA2	1:C:189:ALA:HB2	1.65	0.78
1:C:110:SER:OG	1:C:112:ILE:CG2	2.31	0.78
1:C:115:VAL:HG13	1:C:119:ASP:HB2	1.63	0.78
1:C:110:SER:OG	1:C:112:ILE:HG22	1.85	0.77
1:A:172:ILE:CG2	1:B:143:PRO:HG3	2.14	0.77
1:B:33:MET:HE1	1:C:14:LYS:HE3	1.66	0.77
1:D:117:PRO:O	1:D:120:ILE:HG12	1.85	0.77
1:C:83:VAL:HG13	1:C:84:SER:N	1.94	0.76
1:C:67:CYS:SG	1:C:70:CYS:HB2	2.26	0.76
1:A:160:PRO:HG2	4:A:315:HOH:O	1.86	0.75
1:C:58:CYS:SG	1:C:60:ASN:HB2	2.28	0.74
1:B:21:LYS:HB3	4:B:308:HOH:O	1.86	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2:SER:CB	4:A:319:HOH:O	2.35	0.74
1:B:146:GLU:OE2	1:B:146:GLU:HA	1.87	0.73
1:B:139:LEU:HD23	1:B:166:THR:O	1.88	0.73
1:A:9:ILE:CD1	1:A:24:GLN:HA	2.19	0.73
1:A:62:THR:HG22	1:A:63:ASP:H	1.53	0.73
1:D:15:LEU:CB	1:D:18:ILE:HG13	2.12	0.73
1:B:15:LEU:HD13	1:C:26:LEU:HD22	1.70	0.73
1:C:56:LYS:HE2	4:C:311:HOH:O	1.88	0.73
1:B:139:LEU:HD23	1:B:139:LEU:H	1.54	0.73
1:A:66:VAL:HG23	1:A:71:SER:HB3	1.72	0.72
1:A:9:ILE:HD12	1:A:24:GLN:HA	1.71	0.72
1:D:120:ILE:HD11	1:D:122:ILE:HD12	1.71	0.72
1:A:177:ASP:OD1	1:A:177:ASP:C	2.33	0.71
1:A:38:VAL:HG21	1:D:49:LYS:HG3	1.72	0.71
1:C:83:VAL:CG1	1:C:84:SER:N	2.53	0.71
1:C:78:SER:HB3	1:C:135:LYS:HG2	1.72	0.71
1:D:121:ARG:HG3	1:D:121:ARG:NH1	2.02	0.71
1:C:192:GLY:O	1:C:194:ARG:HG3	1.91	0.71
1:B:97:GLU:HB3	4:B:324:HOH:O	1.90	0.70
1:A:72:ASP:OD1	1:A:72:ASP:C	2.34	0.70
1:C:61:ILE:HD12	1:C:86:PRO:HG2	1.74	0.69
1:D:43:GLN:HG3	4:D:317:HOH:O	1.91	0.69
1:C:11:GLU:HA	1:C:11:GLU:OE1	1.92	0.69
1:A:121:ARG:HH11	1:A:121:ARG:CG	2.06	0.69
1:C:143:PRO:HG3	1:D:172:ILE:HG22	1.75	0.69
1:A:195:GLU:O	1:A:196:VAL:CG2	2.40	0.68
1:B:85:HIS:CE1	1:B:87:MET:HG3	2.28	0.68
1:A:12:LEU:O	1:A:18:ILE:HD11	1.91	0.68
1:C:159:LYS:HD3	1:C:160:PRO:HD3	1.73	0.68
1:A:172:ILE:HG21	1:B:143:PRO:HG3	1.74	0.67
1:C:196:VAL:HG23	1:D:167:ARG:HB2	1.75	0.67
1:D:121:ARG:HH11	1:D:121:ARG:CG	2.05	0.67
1:D:141:THR:OG1	1:D:151:ALA:HB2	1.94	0.67
1:B:22:THR:O	1:B:26:LEU:HB2	1.95	0.67
1:C:87:MET:HA	1:C:90:VAL:HG23	1.77	0.67
1:B:21:LYS:HG3	1:B:22:THR:N	2.10	0.66
1:C:172:ILE:CG2	1:D:143:PRO:HG3	2.25	0.66
1:D:85:HIS:CE1	1:D:87:MET:HE2	2.30	0.66
1:C:67:CYS:HB3	4:C:312:HOH:O	1.95	0.66
1:A:6:ALA:O	1:A:9:ILE:HB	1.97	0.65
1:A:168:ILE:HD11	1:B:190:LEU:CA	2.22	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:167:ARG:HB2	1:B:196:VAL:HG23	1.78	0.65
1:A:124:GLU:H	1:A:124:GLU:CD	2.04	0.65
1:C:67:CYS:SG	1:C:70:CYS:CB	2.84	0.65
1:D:13:SER:HA	1:D:18:ILE:HG22	1.77	0.65
1:B:15:LEU:HB3	1:C:26:LEU:HD21	1.77	0.65
1:C:109:ILE:HG13	1:C:150:THR:HG23	1.77	0.64
1:D:34:PRO:HB3	4:D:315:HOH:O	1.97	0.64
1:D:56:LYS:HG2	1:D:65:GLU:O	1.97	0.64
1:C:196:VAL:CG2	1:D:167:ARG:HB2	2.28	0.64
1:D:120:ILE:HD11	1:D:122:ILE:CD1	2.26	0.64
1:C:19:GLY:O	1:C:22:THR:N	2.30	0.63
1:C:99:LYS:HE2	1:C:99:LYS:H	1.64	0.63
1:B:142:ASN:O	1:B:147:GLY:HA3	1.98	0.63
1:D:78:SER:HA	1:D:134:VAL:HG22	1.81	0.63
1:B:144:ASP:HB2	1:B:146:GLU:HB2	1.81	0.63
1:D:53:ARG:CG	4:D:332:HOH:O	2.46	0.63
1:A:159:LYS:HG3	1:A:160:PRO:HD3	1.81	0.62
1:A:121:ARG:HH11	1:A:121:ARG:HG3	1.63	0.62
1:D:108:VAL:HG13	1:D:150:THR:OG1	1.99	0.62
1:A:60:ASN:HB3	1:A:67:CYS:SG	2.40	0.62
1:C:105:LEU:HB3	1:C:120:ILE:CG2	2.30	0.62
1:B:48:ALA:HB1	1:C:31:ILE:HD11	1.82	0.61
1:B:4:SER:OG	1:C:48:ALA:HA	2.00	0.61
1:C:83:VAL:HG22	1:C:88:ASP:HB3	1.82	0.61
1:C:133:SER:HB3	4:C:313:HOH:O	1.99	0.61
1:A:43:GLN:O	1:A:46:ILE:HG22	2.00	0.61
1:B:3:THR:O	1:B:6:ALA:N	2.33	0.61
1:A:2:SER:HB2	4:A:319:HOH:O	1.99	0.61
1:A:115:VAL:HG13	1:A:119:ASP:HB2	1.83	0.61
1:D:13:SER:CA	1:D:18:ILE:HG21	2.19	0.61
1:D:17:GLY:N	4:D:307:HOH:O	2.25	0.60
1:B:108:VAL:HG12	1:B:109:ILE:H	1.67	0.60
1:D:12:LEU:O	1:D:18:ILE:HG21	2.02	0.60
1:A:67:CYS:C	1:A:69:ILE:H	2.10	0.60
1:D:93:GLU:HA	4:D:302:HOH:O	2.01	0.60
1:D:117:PRO:O	1:D:120:ILE:CG1	2.49	0.60
1:C:122:ILE:O	1:C:126:LEU:HD22	2.02	0.60
1:D:120:ILE:CD1	1:D:122:ILE:CD1	2.80	0.59
1:C:143:PRO:HG3	1:D:172:ILE:CG2	2.32	0.59
1:D:40:SER:HA	4:D:316:HOH:O	2.01	0.59
1:A:180:TYR:OH	1:C:21:LYS:CD	2.48	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:90:VAL:O	1:B:94:LYS:HG3	2.03	0.59
1:B:61:ILE:HG22	1:B:61:ILE:O	2.02	0.59
1:D:111:PRO:O	1:D:112:ILE:HG13	2.01	0.59
1:B:13:SER:HB3	1:B:23:ALA:HB2	1.85	0.59
1:B:109:ILE:O	1:B:109:ILE:CG1	2.40	0.59
1:C:67:CYS:SG	1:C:70:CYS:N	2.72	0.59
1:B:52:LEU:HD21	1:B:54:TYR:HE2	1.68	0.59
1:C:109:ILE:HD12	1:C:150:THR:HA	1.83	0.59
1:A:161:PHE:CD1	1:A:161:PHE:N	2.71	0.59
1:A:190:LEU:HD22	1:B:92:MET:HE1	1.84	0.59
1:D:43:GLN:O	1:D:44:ALA:C	2.45	0.59
1:D:64:LYS:HE3	1:D:68:ASP:OD1	2.03	0.59
1:A:33:MET:O	1:D:49:LYS:HE3	2.03	0.58
1:A:1:TYR:OH	1:D:87:MET:HG2	2.03	0.58
1:A:121:ARG:HG3	1:A:121:ARG:NH1	2.17	0.58
1:C:172:ILE:HG22	1:D:143:PRO:HG3	1.85	0.58
1:D:161:PHE:HD1	1:D:161:PHE:H	1.50	0.58
1:B:153:TYR:O	1:B:156:LYS:HB2	2.03	0.58
1:C:3:THR:O	1:C:7:LYS:HB2	2.03	0.58
1:D:21:LYS:HB3	4:D:314:HOH:O	2.03	0.58
1:A:196:VAL:HG23	1:A:196:VAL:OXT	2.03	0.58
1:D:-2:MET:H2	1:D:1:TYR:HE2	1.48	0.58
1:C:67:CYS:SG	1:C:70:CYS:SG	3.01	0.58
1:A:76:ASP:OD2	1:A:79:THR:HG23	2.03	0.58
1:D:121:ARG:NH1	1:D:121:ARG:HA	2.19	0.58
1:A:125:LEU:O	1:A:129:VAL:HG12	2.04	0.58
1:A:166:THR:HA	1:B:195:GLU:HA	1.84	0.58
1:B:157:LEU:O	1:B:160:PRO:HD2	2.04	0.58
1:C:115:VAL:HG12	1:C:116:GLY:N	2.18	0.58
1:B:92:MET:O	1:B:95:VAL:HG22	2.04	0.57
1:D:59:PHE:CZ	1:D:124:GLU:HG3	2.39	0.57
1:D:103:HIS:HB2	1:D:128:ARG:HH11	1.67	0.57
1:A:122:ILE:CG2	1:A:123:LYS:HD3	2.28	0.57
1:C:189:ALA:HA	1:D:169:ALA:HB3	1.85	0.57
1:B:13:SER:HB3	1:B:23:ALA:CB	2.34	0.57
1:B:118:GLU:HB3	4:B:334:HOH:O	2.03	0.57
1:D:10:GLU:O	1:D:14:LYS:HG3	2.05	0.57
1:B:74:ASN:HA	4:B:323:HOH:O	2.04	0.57
1:C:9:ILE:HD13	1:C:24:GLN:HG2	1.86	0.57
1:C:127:GLU:HG2	1:C:130:ARG:HH12	1.68	0.57
1:D:131:ASP:OD1	1:D:131:ASP:N	2.22	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:161:PHE:CD1	1:D:161:PHE:N	2.73	0.57
1:A:2:SER:HB3	4:A:319:HOH:O	2.02	0.57
1:B:195:GLU:O	1:B:196:VAL:C	2.48	0.56
1:C:49:LYS:O	1:C:49:LYS:HG3	2.05	0.56
1:D:22:THR:O	1:D:26:LEU:HB2	2.06	0.56
1:A:142:ASN:CG	1:B:177:ASP:HB2	2.30	0.56
1:D:112:ILE:HG22	1:D:113:GLU:N	2.21	0.56
1:C:155:ALA:C	1:C:157:LEU:H	2.13	0.56
1:D:74:ASN:OD1	1:D:74:ASN:N	2.39	0.56
1:A:143:PRO:HD2	1:B:176:GLY:O	2.06	0.56
1:C:59:PHE:CD1	1:C:59:PHE:N	2.73	0.56
1:A:172:ILE:HG22	1:B:143:PRO:HG3	1.88	0.56
1:C:62:THR:OG1	1:C:63:ASP:N	2.34	0.56
1:C:18:ILE:HG22	1:C:18:ILE:O	2.05	0.56
1:C:146:GLU:O	1:C:149:ALA:N	2.38	0.55
1:C:18:ILE:O	1:C:18:ILE:CG2	2.55	0.55
1:C:159:LYS:N	1:C:160:PRO:CD	2.69	0.55
1:C:69:ILE:HG23	1:C:75:ARG:HD2	1.89	0.55
1:D:142:ASN:O	1:D:147:GLY:HA3	2.07	0.55
1:A:67:CYS:C	1:A:69:ILE:N	2.63	0.55
1:B:27:ALA:O	1:B:30:ILE:HB	2.07	0.55
1:C:107:GLY:HA3	1:C:120:ILE:HD12	1.87	0.55
1:A:167:ARG:HG3	1:A:167:ARG:HH11	1.71	0.55
1:B:34:PRO:HA	4:B:310:HOH:O	2.08	0.54
1:B:7:LYS:O	1:B:8:LEU:C	2.49	0.54
1:C:189:ALA:CA	1:D:169:ALA:HB3	2.38	0.54
1:A:58:CYS:SG	1:A:60:ASN:HB2	2.48	0.54
1:B:115:VAL:HG12	1:B:116:GLY:H	1.71	0.54
1:C:37:GLU:HA	1:C:40:SER:HB2	1.90	0.54
1:C:5:VAL:HG22	1:C:31:ILE:CD1	2.38	0.54
1:C:12:LEU:O	1:C:18:ILE:HG21	2.07	0.54
1:D:174:VAL:HG12	1:D:174:VAL:O	2.07	0.54
1:C:170:HIS:HB3	1:D:174:VAL:HG23	1.89	0.54
1:D:159:LYS:O	1:D:160:PRO:C	2.51	0.54
1:A:59:PHE:CD1	1:A:121:ARG:HG2	2.42	0.53
1:B:21:LYS:CG	1:B:22:THR:H	2.20	0.53
1:D:121:ARG:HH11	1:D:121:ARG:HA	1.73	0.53
1:C:172:ILE:HG21	1:D:143:PRO:HG3	1.89	0.53
1:B:144:ASP:HB3	4:B:314:HOH:O	2.07	0.53
1:A:113:GLU:HA	1:A:113:GLU:OE1	2.07	0.53
1:A:5:VAL:O	1:A:9:ILE:HG12	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:159:LYS:N	1:C:160:PRO:HD2	2.24	0.53
1:D:103:HIS:C	1:D:103:HIS:CD2	2.86	0.52
1:D:194:ARG:HD2	4:D:311:HOH:O	2.10	0.52
1:C:38:VAL:HG12	1:C:38:VAL:O	2.09	0.52
1:A:18:ILE:O	1:A:18:ILE:CG1	2.55	0.52
1:C:83:VAL:CG2	1:C:88:ASP:HB3	2.39	0.52
1:B:110:SER:HB2	1:B:112:ILE:HG22	1.92	0.52
1:B:110:SER:HB3	1:B:146:GLU:OE1	2.09	0.52
1:A:26:LEU:HD22	1:D:15:LEU:HD12	1.92	0.51
1:A:59:PHE:CE1	1:A:121:ARG:NH1	2.78	0.51
1:D:28:PHE:HA	1:D:31:ILE:HG12	1.93	0.51
1:D:142:ASN:HB2	1:D:144:ASP:OD1	2.09	0.51
1:A:66:VAL:CG2	1:A:71:SER:HB3	2.39	0.51
1:A:103:HIS:HB2	1:A:128:ARG:NH1	2.25	0.51
1:C:146:GLU:O	1:C:147:GLY:C	2.53	0.51
1:D:-2:MET:HG2	1:D:-1:SER:H	1.74	0.51
1:D:59:PHE:CE1	1:D:124:GLU:HB2	2.45	0.51
1:B:11:GLU:OE2	1:C:41:LEU:HA	2.10	0.51
1:B:15:LEU:HD11	1:C:30:ILE:HD11	1.93	0.51
1:A:67:CYS:O	1:A:69:ILE:N	2.44	0.51
1:A:192:GLY:O	1:A:193:ARG:C	2.54	0.51
1:C:5:VAL:O	1:C:9:ILE:HG13	2.11	0.51
1:B:108:VAL:HG12	1:B:150:THR:OG1	2.11	0.51
1:D:-2:MET:HE2	1:D:-2:MET:N	2.25	0.51
1:C:117:PRO:HG3	1:C:153:TYR:CZ	2.45	0.51
1:A:161:PHE:HD1	1:A:161:PHE:H	1.59	0.51
1:B:52:LEU:HD21	1:B:54:TYR:CE2	2.46	0.50
1:B:153:TYR:C	1:B:156:LYS:H	2.19	0.50
1:D:103:HIS:CB	1:D:128:ARG:NH1	2.71	0.50
1:A:81:CYS:HB2	1:A:98:TYR:CZ	2.47	0.50
1:A:167:ARG:HG3	1:A:168:ILE:N	2.26	0.50
1:D:53:ARG:HG2	4:D:332:HOH:O	2.09	0.50
1:A:121:ARG:CG	1:A:121:ARG:NH1	2.71	0.50
1:B:59:PHE:CE1	1:B:124:GLU:HB2	2.46	0.50
1:B:76:ASP:C	1:B:78:SER:H	2.19	0.50
1:C:124:GLU:O	1:C:128:ARG:HG3	2.12	0.50
1:D:8:LEU:HD12	1:D:8:LEU:O	2.11	0.50
1:D:108:VAL:HG11	1:D:146:GLU:HB3	1.93	0.50
1:B:40:SER:O	1:B:41:LEU:C	2.51	0.50
1:C:13:SER:HA	1:C:18:ILE:CG2	2.42	0.50
1:C:36:ASP:O	1:C:40:SER:HB2	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:39:ARG:O	1:C:40:SER:C	2.55	0.50
1:C:79:THR:HG22	1:C:136:GLU:HB3	1.92	0.50
1:D:109:ILE:HD12	1:D:150:THR:HA	1.93	0.50
1:C:72:ASP:C	4:C:323:HOH:O	2.54	0.49
1:D:123:LYS:HB3	1:D:124:GLU:OE1	2.12	0.49
1:B:85:HIS:CE1	1:B:87:MET:CG	2.95	0.49
1:C:78:SER:CB	1:C:135:LYS:HG2	2.42	0.49
1:A:13:SER:N	1:A:18:ILE:HD11	2.28	0.49
1:C:73:GLU:N	4:C:323:HOH:O	2.46	0.49
1:B:129:VAL:HG22	1:B:129:VAL:O	2.13	0.49
1:A:103:HIS:NE2	1:A:121:ARG:O	2.39	0.49
1:A:41:LEU:O	1:A:42:SER:C	2.55	0.49
1:C:30:ILE:HG22	1:C:31:ILE:N	2.28	0.49
1:C:110:SER:OG	1:C:112:ILE:HG23	2.13	0.49
1:C:122:ILE:HG22	1:C:123:LYS:N	2.25	0.49
1:C:37:GLU:C	1:C:39:ARG:N	2.70	0.48
1:C:58:CYS:SG	1:C:60:ASN:CB	3.01	0.48
1:A:123:LYS:CB	4:A:312:HOH:O	2.61	0.48
1:B:151:ALA:O	1:B:153:TYR:N	2.47	0.48
1:C:73:GLU:CA	4:C:323:HOH:O	2.60	0.48
1:C:1:TYR:CD2	1:C:28:PHE:HZ	2.31	0.48
1:C:183:VAL:O	1:C:187:SER:N	2.26	0.48
1:D:53:ARG:HG3	4:D:332:HOH:O	2.08	0.48
1:D:58:CYS:HB2	1:D:102:TYR:O	2.13	0.48
1:A:120:ILE:O	1:A:122:ILE:N	2.45	0.48
1:A:30:ILE:O	1:A:33:MET:CG	2.62	0.48
1:B:9:ILE:O	1:B:10:GLU:C	2.56	0.48
1:C:123:LYS:O	1:C:127:GLU:HG3	2.13	0.48
1:B:112:ILE:O	1:B:112:ILE:HG13	2.13	0.48
1:A:1:TYR:CD1	1:A:28:PHE:HZ	2.32	0.48
1:C:186:LEU:O	1:C:187:SER:C	2.57	0.48
1:D:110:SER:C	1:D:112:ILE:H	2.22	0.48
1:B:86:PRO:HD3	1:B:104:VAL:HG11	1.95	0.48
1:A:91:ALA:O	1:A:93:GLU:N	2.47	0.47
1:C:6:ALA:HA	1:C:9:ILE:HD12	1.96	0.47
1:D:98:TYR:CZ	1:D:100:GLY:HA3	2.49	0.47
1:A:30:ILE:O	1:A:33:MET:HG2	2.14	0.47
1:A:121:ARG:HD2	1:A:121:ARG:N	2.29	0.47
1:C:105:LEU:HB3	1:C:120:ILE:HG22	1.95	0.47
1:D:145:ILE:HD12	1:D:145:ILE:H	1.79	0.47
1:C:127:GLU:HG2	1:C:130:ARG:NH1	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:92:MET:HB3	1:C:102:TYR:OH	2.15	0.47
1:C:173:PRO:HD3	1:D:173:PRO:HG3	1.95	0.47
1:D:120:ILE:O	1:D:121:ARG:NH1	2.48	0.47
1:D:-2:MET:CG	1:D:-1:SER:H	2.27	0.47
1:C:67:CYS:C	1:C:69:ILE:H	2.22	0.47
1:D:113:GLU:HA	4:D:319:HOH:O	2.14	0.46
1:B:20:PRO:O	1:B:21:LYS:C	2.57	0.46
1:B:139:LEU:HD21	1:B:165:VAL:HG12	1.97	0.46
1:C:47:GLU:O	1:C:48:ALA:C	2.57	0.46
1:D:-2:MET:HE2	1:D:-2:MET:H1	1.81	0.46
1:A:186:LEU:HB3	1:B:95:VAL:HG11	1.97	0.46
1:B:103:HIS:CE1	1:B:125:LEU:HA	2.50	0.46
1:C:72:ASP:OD1	1:C:73:GLU:N	2.48	0.46
1:C:123:LYS:O	4:C:321:HOH:O	2.20	0.46
1:A:126:LEU:O	1:A:130:ARG:N	2.45	0.46
1:B:161:PHE:N	1:B:161:PHE:CD2	2.84	0.46
1:D:25:ARG:NH1	1:D:25:ARG:CG	2.70	0.46
1:D:112:ILE:CG2	1:D:113:GLU:N	2.79	0.46
1:A:21:LYS:HG2	4:A:318:HOH:O	2.15	0.46
1:A:92:MET:HE1	1:B:190:LEU:HD13	1.98	0.46
1:B:129:VAL:HG23	1:B:134:VAL:HG22	1.97	0.46
1:A:34:PRO:HG2	1:A:37:GLU:CD	2.41	0.46
1:B:82:VAL:HG12	1:B:83:VAL:N	2.31	0.46
1:C:155:ALA:C	1:C:157:LEU:N	2.74	0.46
1:B:188:LYS:O	1:B:189:ALA:C	2.59	0.46
1:A:157:LEU:HD23	1:A:157:LEU:HA	1.47	0.45
1:B:81:CYS:HB2	1:B:98:TYR:CZ	2.51	0.45
1:B:110:SER:HA	4:B:322:HOH:O	2.15	0.45
1:C:112:ILE:HG23	1:C:113:GLU:N	2.31	0.45
1:B:46:ILE:HD11	1:C:39:ARG:HG3	1.98	0.45
1:C:58:CYS:C	1:C:59:PHE:HD1	2.24	0.45
1:D:15:LEU:HD22	1:D:15:LEU:N	2.30	0.45
1:D:108:VAL:HG12	1:D:109:ILE:N	2.30	0.45
1:D:95:VAL:HG12	1:D:97:GLU:HB2	1.98	0.45
1:A:10:GLU:HA	1:A:13:SER:OG	2.16	0.45
1:A:29:PHE:C	1:A:29:PHE:CD2	2.94	0.45
1:A:129:VAL:HA	1:A:134:VAL:HG21	1.98	0.45
1:B:16:PRO:HD2	1:C:26:LEU:CD2	2.47	0.45
1:D:57:ILE:HD12	1:D:70:CYS:HB3	1.99	0.45
1:D:69:ILE:HD12	1:D:75:ARG:HH12	1.82	0.45
1:C:95:VAL:HG12	1:C:97:GLU:HG2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:21:LYS:HG3	1:A:22:THR:N	2.31	0.45
1:A:177:ASP:OD1	1:A:177:ASP:O	2.33	0.45
1:D:83:VAL:HG13	1:D:84:SER:N	2.32	0.45
1:D:135:LYS:HG2	4:D:322:HOH:O	2.15	0.45
1:A:169:ALA:HB2	1:B:192:GLY:O	2.17	0.45
1:B:16:PRO:HD2	1:C:26:LEU:HD21	1.98	0.45
1:C:183:VAL:HG13	1:D:95:VAL:HA	1.99	0.45
1:D:146:GLU:O	1:D:147:GLY:C	2.60	0.44
1:A:34:PRO:O	1:A:38:VAL:HG23	2.16	0.44
1:B:156:LYS:O	1:B:159:LYS:HB3	2.17	0.44
1:D:30:ILE:HA	1:D:33:MET:SD	2.57	0.44
1:C:37:GLU:C	1:C:39:ARG:H	2.25	0.44
1:C:156:LYS:HE3	1:C:156:LYS:CA	2.48	0.44
1:D:135:LYS:C	1:D:163:VAL:HG13	2.42	0.44
1:B:19:GLY:N	1:B:22:THR:OG1	2.51	0.44
1:C:189:ALA:CB	1:D:169:ALA:HB3	2.48	0.44
1:B:49:LYS:CG	1:C:35:LEU:CD2	2.96	0.44
1:C:8:LEU:O	1:C:9:ILE:C	2.59	0.44
1:C:13:SER:HA	1:C:18:ILE:HG21	1.99	0.44
1:C:73:GLU:HA	1:C:77:HIS:HE2	1.82	0.44
1:C:136:GLU:HG3	1:C:164:LYS:O	2.18	0.44
1:D:59:PHE:CZ	1:D:124:GLU:HB2	2.52	0.44
1:D:56:LYS:HA	1:D:56:LYS:HD3	1.66	0.44
1:D:120:ILE:HD12	1:D:122:ILE:HG13	1.98	0.44
1:D:194:ARG:CD	4:D:311:HOH:O	2.66	0.44
1:A:117:PRO:HD2	4:A:311:HOH:O	2.18	0.44
1:A:8:LEU:HG	1:A:12:LEU:CD1	2.47	0.44
1:C:12:LEU:HD12	1:C:12:LEU:HA	1.64	0.44
1:D:33:MET:CE	1:D:37:GLU:HB3	2.48	0.44
1:A:3:THR:N	4:A:319:HOH:O	2.33	0.43
1:B:79:THR:HA	1:B:136:GLU:O	2.17	0.43
1:B:146:GLU:OE2	1:B:146:GLU:CA	2.61	0.43
1:A:34:PRO:HB2	1:A:36:ASP:OD2	2.18	0.43
1:B:153:TYR:C	1:B:155:ALA:N	2.72	0.43
1:B:73:GLU:HG2	4:B:319:HOH:O	2.17	0.43
1:B:33:MET:HE2	1:B:37:GLU:HB3	2.01	0.43
1:A:122:ILE:O	1:A:125:LEU:HB3	2.18	0.43
1:B:110:SER:HB2	1:B:112:ILE:CG2	2.49	0.43
1:C:12:LEU:O	1:C:15:LEU:HB2	2.18	0.43
1:D:110:SER:C	1:D:112:ILE:N	2.76	0.43
1:A:79:THR:HA	1:A:136:GLU:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:126:LEU:O	1:C:129:VAL:HG12	2.19	0.43
1:D:78:SER:OG	1:D:135:LYS:HE3	2.18	0.43
1:A:8:LEU:O	1:A:9:ILE:C	2.62	0.43
1:A:103:HIS:HD2	1:A:105:LEU:HD23	1.83	0.43
1:A:173:PRO:HA	1:B:185:THR:HG23	2.01	0.43
1:A:47:GLU:HG2	1:A:51:LYS:NZ	2.33	0.43
1:A:179:GLU:OE1	1:B:87:MET:HB3	2.18	0.43
1:C:155:ALA:O	1:C:157:LEU:N	2.42	0.43
1:C:196:VAL:HG11	1:D:155:ALA:HB1	2.01	0.43
1:B:15:LEU:HD23	1:B:15:LEU:HA	1.74	0.43
1:D:92:MET:O	1:D:95:VAL:HB	2.19	0.43
1:C:43:GLN:O	1:C:44:ALA:C	2.61	0.42
1:C:72:ASP:O	1:C:77:HIS:NE2	2.52	0.42
1:C:115:VAL:CG1	1:C:116:GLY:N	2.81	0.42
1:D:58:CYS:SG	1:D:60:ASN:HB2	2.59	0.42
1:C:159:LYS:HE2	1:C:159:LYS:HB2	1.70	0.42
1:A:195:GLU:C	1:A:196:VAL:HG22	2.38	0.42
1:B:191:GLU:O	1:B:191:GLU:HG2	2.18	0.42
1:B:5:VAL:C	1:B:7:LYS:H	2.27	0.42
1:B:28:PHE:O	1:B:29:PHE:C	2.62	0.42
1:C:126:LEU:HD22	1:C:126:LEU:H	1.84	0.42
1:A:88:ASP:O	1:A:91:ALA:HB3	2.20	0.42
1:B:49:LYS:HG3	1:C:35:LEU:HD21	2.01	0.42
1:B:109:ILE:CD1	1:B:149:ALA:HB1	2.38	0.42
1:C:15:LEU:N	1:C:15:LEU:CD2	2.82	0.42
1:A:5:VAL:O	1:A:6:ALA:C	2.61	0.42
1:B:151:ALA:C	1:B:153:TYR:N	2.78	0.42
1:B:81:CYS:HB2	1:B:98:TYR:OH	2.20	0.42
1:B:115:VAL:HG13	1:B:119:ASP:HB2	2.02	0.42
1:C:171:GLY:CA	1:C:189:ALA:HB2	2.45	0.42
1:D:26:LEU:HD23	1:D:26:LEU:HA	1.74	0.42
1:B:49:LYS:HG3	1:C:35:LEU:CD2	2.50	0.42
1:D:74:ASN:ND2	4:D:334:HOH:O	2.52	0.42
1:A:8:LEU:HG	1:A:12:LEU:HD11	2.02	0.42
1:C:10:GLU:O	1:C:13:SER:N	2.51	0.42
1:C:154:ILE:O	1:C:158:LEU:HB3	2.20	0.42
1:B:103:HIS:NE2	1:B:125:LEU:HB2	2.35	0.41
1:B:153:TYR:O	1:B:156:LYS:N	2.51	0.41
1:A:0:TYR:N	1:D:90:VAL:HG11	2.35	0.41
1:A:76:ASP:OD1	1:A:78:SER:HB2	2.21	0.41
1:B:71:SER:O	1:B:72:ASP:C	2.63	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:168:ILE:HA	1:B:168:ILE:HD12	1.64	0.41
1:B:194:ARG:O	1:B:195:GLU:C	2.63	0.41
1:C:59:PHE:CD2	1:C:121:ARG:HD3	2.56	0.41
1:C:75:ARG:NH2	1:C:93:GLU:OE1	2.51	0.41
1:D:122:ILE:O	1:D:123:LYS:C	2.62	0.41
1:D:159:LYS:HB3	1:D:160:PRO:CD	2.51	0.41
1:A:9:ILE:HG22	1:A:10:GLU:N	2.35	0.41
1:A:95:VAL:HG13	1:B:187:SER:HB2	2.02	0.41
1:A:115:VAL:HG13	1:A:119:ASP:CB	2.50	0.41
1:C:182:ASP:O	1:C:183:VAL:C	2.63	0.41
1:D:108:VAL:CG1	1:D:109:ILE:N	2.83	0.41
1:B:120:ILE:O	1:B:122:ILE:N	2.50	0.41
1:B:139:LEU:HD23	1:B:139:LEU:N	2.27	0.41
1:D:83:VAL:HG13	1:D:85:HIS:H	1.86	0.41
1:D:139:LEU:HD23	1:D:139:LEU:HA	1.12	0.41
1:A:26:LEU:HD23	1:D:16:PRO:HD2	2.02	0.41
1:B:33:MET:O	1:C:49:LYS:HE2	2.21	0.41
1:D:21:LYS:HB2	1:D:25:ARG:HH22	1.86	0.41
1:D:157:LEU:HD23	1:D:157:LEU:HA	1.68	0.41
1:B:15:LEU:CD1	1:C:30:ILE:HD11	2.51	0.41
1:C:159:LYS:CD	1:C:160:PRO:HD3	2.47	0.41
1:D:12:LEU:O	1:D:15:LEU:HD23	2.20	0.41
1:A:9:ILE:HD13	1:A:27:ALA:CB	2.50	0.41
1:A:66:VAL:HG23	1:A:66:VAL:O	2.20	0.41
1:A:103:HIS:CD2	1:A:105:LEU:HD23	2.55	0.41
1:A:168:ILE:HD12	1:A:168:ILE:HA	1.61	0.41
1:A:168:ILE:CG2	1:B:172:ILE:HD11	2.50	0.41
1:D:181:THR:HG23	1:D:185:THR:CG2	2.51	0.41
1:A:168:ILE:HG23	1:B:172:ILE:CD1	2.51	0.41
1:B:2:SER:OG	1:B:3:THR:N	2.32	0.41
1:B:5:VAL:C	1:B:7:LYS:N	2.79	0.41
1:B:15:LEU:HD13	1:C:26:LEU:CD2	2.47	0.41
1:B:28:PHE:CD1	3:B:202:IMD:H2	2.56	0.41
1:D:112:ILE:CG2	1:D:113:GLU:H	2.34	0.41
1:D:146:GLU:HB2	1:D:147:GLY:H	1.73	0.41
1:A:108:VAL:HG21	1:A:146:GLU:HG3	2.03	0.41
1:B:88:ASP:O	1:B:91:ALA:HB3	2.20	0.41
1:B:94:LYS:C	1:B:96:LYS:N	2.79	0.41
1:B:194:ARG:O	1:B:196:VAL:N	2.54	0.40
1:D:103:HIS:HB2	1:D:128:ARG:HH12	1.80	0.40
1:A:41:LEU:O	1:A:43:GLN:N	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:129:VAL:O	1:B:129:VAL:CG2	2.68	0.40
1:A:173:PRO:HA	1:B:185:THR:CG2	2.51	0.40
1:B:108:VAL:CG1	1:B:150:THR:OG1	2.70	0.40
1:D:181:THR:HG23	1:D:185:THR:HG21	2.03	0.40
1:A:98:TYR:CZ	1:A:100:GLY:HA3	2.56	0.40
1:B:99:LYS:HD3	1:B:99:LYS:N	2.36	0.40
1:B:108:VAL:HG12	1:B:109:ILE:N	2.35	0.40
1:C:143:PRO:HB2	1:D:174:VAL:HA	2.03	0.40
1:D:188:LYS:HE2	1:D:188:LYS:HB2	1.96	0.40
1:A:41:LEU:O	1:A:44:ALA:N	2.54	0.40
1:C:26:LEU:HD23	1:C:26:LEU:HA	1.84	0.40
1:C:146:GLU:HA	1:C:149:ALA:HB3	2.04	0.40
1:C:159:LYS:H	1:C:160:PRO:HD2	1.85	0.40
1:C:195:GLU:HA	1:D:166:THR:HA	2.04	0.40
1:D:34:PRO:O	1:D:37:GLU:HB2	2.21	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	195/212 (92%)	166 (85%)	19 (10%)	10 (5%)	1	10
1	B	195/212 (92%)	146 (75%)	35 (18%)	14 (7%)	1	4
1	C	195/212 (92%)	149 (76%)	34 (17%)	12 (6%)	1	6
1	D	197/212 (93%)	167 (85%)	25 (13%)	5 (2%)	4	23
All	All	782/848 (92%)	628 (80%)	113 (14%)	41 (5%)	1	9

All (41) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	91	ALA
1	A	92	MET
1	B	3	THR
1	B	4	SER
1	B	21	LYS
1	B	71	SER
1	B	72	ASP
1	B	112	ILE
1	B	195	GLU
1	C	117	PRO
1	A	2	SER
1	A	9	ILE
1	B	149	ALA
1	C	42	SER
1	C	183	VAL
1	A	42	SER
1	A	121	ARG
1	A	193	ARG
1	B	146	GLU
1	C	36	ASP
1	C	68	ASP
1	C	156	LYS
1	C	164	LYS
1	D	146	GLU
1	D	195	GLU
1	A	41	LEU
1	A	68	ASP
1	B	83	VAL
1	C	10	GLU
1	C	40	SER
1	C	157	LEU
1	D	147	GLY
1	D	174	VAL
1	B	77	HIS
1	B	96	LYS
1	B	152	MET
1	C	20	PRO
1	D	160	PRO
1	B	20	PRO
1	C	147	GLY
1	A	31	ILE

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	167/185 (90%)	139 (83%)	28 (17%)	2	11
1	B	165/185 (89%)	131 (79%)	34 (21%)	1	7
1	C	167/185 (90%)	131 (78%)	36 (22%)	1	6
1	D	165/185 (89%)	128 (78%)	37 (22%)	1	5
All	All	664/740 (90%)	529 (80%)	135 (20%)	1	7

All (135) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	0	TYR
1	A	2	SER
1	A	3	THR
1	A	13	SER
1	A	18	ILE
1	A	22	THR
1	A	32	ASN
1	A	52	LEU
1	A	61	ILE
1	A	62	THR
1	A	67	CYS
1	A	68	ASP
1	A	70	CYS
1	A	72	ASP
1	A	83	VAL
1	A	87	MET
1	A	99	LYS
1	A	112	ILE
1	A	121	ARG
1	A	124	GLU
1	A	158	LEU
1	A	159	LYS
1	A	168	ILE
1	A	172	ILE

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Mol	Chain	Res	Type
1	A	177	ASP
1	A	182	ASP
1	A	183	VAL
1	A	184	VAL
1	B	4	SER
1	B	5	VAL
1	B	22	THR
1	B	24	GLN
1	B	26	LEU
1	B	30	ILE
1	B	36	ASP
1	B	39	ARG
1	B	43	GLN
1	B	46	ILE
1	B	57	ILE
1	B	68	ASP
1	B	71	SER
1	B	79	THR
1	B	90	VAL
1	B	99	LYS
1	B	108	VAL
1	B	115	VAL
1	B	118	GLU
1	B	120	ILE
1	B	124	GLU
1	B	129	VAL
1	B	135	LYS
1	B	139	LEU
1	B	146	GLU
1	B	153	TYR
1	B	156	LYS
1	B	159	LYS
1	B	168	ILE
1	B	172	ILE
1	B	184	VAL
1	B	190	LEU
1	B	191	GLU
1	B	196	VAL
1	C	3	THR
1	C	13	SER
1	C	15	LEU
1	C	18	ILE

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Mol	Chain	Res	Type
1	C	30	ILE
1	C	31	ILE
1	C	32	ASN
1	C	35	LEU
1	C	37	GLU
1	C	40	SER
1	C	56	LYS
1	C	61	ILE
1	C	62	THR
1	C	64	LYS
1	C	67	CYS
1	C	73	GLU
1	C	83	VAL
1	C	84	SER
1	C	87	MET
1	C	90	VAL
1	C	99	LYS
1	C	118	GLU
1	C	121	ARG
1	C	122	ILE
1	C	126	LEU
1	C	129	VAL
1	C	135	LYS
1	C	146	GLU
1	C	148	GLU
1	C	156	LYS
1	C	157	LEU
1	C	159	LYS
1	C	161	PHE
1	C	179	GLU
1	C	184	VAL
1	C	191	GLU
1	D	-2	MET
1	D	1	TYR
1	D	3	THR
1	D	14	LYS
1	D	21	LYS
1	D	22	THR
1	D	25	ARG
1	D	38	VAL
1	D	49	LYS
1	D	53	ARG

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Mol	Chain	Res	Type
1	D	54	TYR
1	D	62	THR
1	D	66	VAL
1	D	71	SER
1	D	74	ASN
1	D	83	VAL
1	D	90	VAL
1	D	121	ARG
1	D	124	GLU
1	D	125	LEU
1	D	126	LEU
1	D	129	VAL
1	D	131	ASP
1	D	135	LYS
1	D	137	VAL
1	D	141	THR
1	D	146	GLU
1	D	157	LEU
1	D	159	LYS
1	D	161	PHE
1	D	166	THR
1	D	174	VAL
1	D	183	VAL
1	D	184	VAL
1	D	186	LEU
1	D	188	LYS
1	D	191	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	170	HIS
1	B	74	ASN
1	C	85	HIS

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	IMD	A	203	-	5,5,5	0.70	0	5,5,5	0.37	0
3	IMD	B	202	-	5,5,5	0.67	0	5,5,5	0.49	0
3	IMD	A	202	-	5,5,5	0.79	0	5,5,5	0.83	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	IMD	A	203	-	-	-	0/1/1/1
3	IMD	B	202	-	-	-	0/1/1/1
3	IMD	A	202	-	-	-	0/1/1/1

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.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	202	IMD	1	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	197/212 (92%)	-0.44	1 (0%) 87 72	31, 70, 101, 139	0
1	B	197/212 (92%)	-0.29	1 (0%) 87 72	42, 78, 125, 158	0
1	C	197/212 (92%)	-0.36	0 100 100	37, 75, 119, 155	0
1	D	199/212 (93%)	-0.27	3 (1%) 72 49	40, 72, 122, 155	0
All	All	790/848 (93%)	-0.34	5 (0%) 85 69	31, 74, 119, 158	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	3	THR	3.7
1	D	120	ILE	2.8
1	D	54	TYR	2.5
1	A	196	VAL	2.5
1	D	55	GLY	2.5

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 oligosaccharides 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
3	IMD	A	202	5/5	0.86	0.15	69,70,70,71	0
3	IMD	B	202	5/5	0.86	0.16	97,98,99,99	0
3	IMD	A	203	5/5	0.91	0.16	67,67,68,69	0
2	ZN	A	201	1/1	0.96	0.05	59,59,59,59	0
2	ZN	D	201	1/1	0.99	0.03	66,66,66,66	0
2	ZN	C	201	1/1	0.99	0.04	75,75,75,75	0
2	ZN	B	201	1/1	1.00	0.01	54,54,54,54	0

6.5 Other polymers [i](#)

There are no such residues in this entry.