Full wwPDB X-ray Structure Validation Report ⓘ

Sep 3, 2023 – 05:40 PM EDT

PDB ID	:	3RTR
Title	:	A RING E3-substrate complex poised for ubiquitin-like protein transfer: structural insights into cullin-RING ligases
Authors	:	Calabrese, M.F.; Scott, D.C.; Duda, D.M.; Grace, C.R.; Kurinov, I.; Kriwacki, R.W.; Schulman, B.A.
Deposited on	:	2011-05-03
Resolution	:	3.21 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:

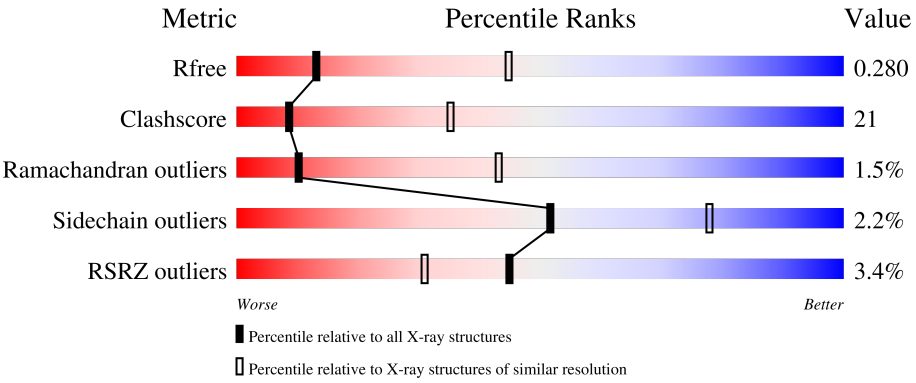
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 3.21 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	1335 (3.24-3.20)
Clashscore	141614	1460 (3.24-3.20)
Ramachandran outliers	138981	1437 (3.24-3.20)
Sidechain outliers	138945	1436 (3.24-3.20)
RSRZ outliers	127900	1291 (3.24-3.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	368	2% 55% 39%
1	C	368	4% 45% 39% 14%
1	E	368	4% 57% 38%
1	G	368	2% 57% 39%
2	B	106	4% 52% 29% 19%

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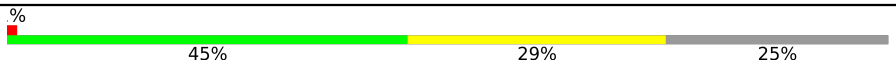
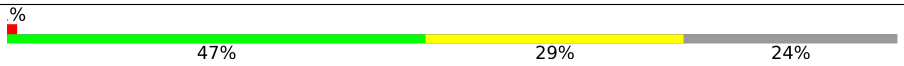
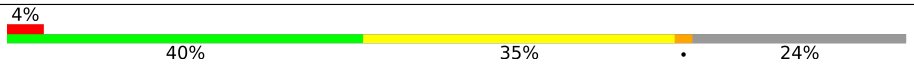
Mol	Chain	Length	Quality of chain
2	D	106	
2	F	106	
2	H	106	

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 14055 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 Cullin-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	353	Total	C	N	O	S	0	0	0
			2870	1822	485	549	14			
1	C	317	Total	C	N	O	S	0	0	0
			2592	1647	439	494	12			
1	E	359	Total	C	N	O	S	0	0	0
			2918	1853	492	560	13			
1	G	360	Total	C	N	O	S	0	0	0
			2937	1866	495	562	14			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	409	GLY	-	expression tag	UNP Q13616
A	410	SER	-	expression tag	UNP Q13616
A	421	GLU	LEU	engineered mutation	UNP Q13616
A	451	GLU	VAL	engineered mutation	UNP Q13616
A	452	LYS	VAL	engineered mutation	UNP Q13616
A	455	LYS	TYR	engineered mutation	UNP Q13616
C	409	GLY	-	expression tag	UNP Q13616
C	410	SER	-	expression tag	UNP Q13616
C	421	GLU	LEU	engineered mutation	UNP Q13616
C	451	GLU	VAL	engineered mutation	UNP Q13616
C	452	LYS	VAL	engineered mutation	UNP Q13616
C	455	LYS	TYR	engineered mutation	UNP Q13616
E	409	GLY	-	expression tag	UNP Q13616
E	410	SER	-	expression tag	UNP Q13616
E	421	GLU	LEU	engineered mutation	UNP Q13616
E	451	GLU	VAL	engineered mutation	UNP Q13616
E	452	LYS	VAL	engineered mutation	UNP Q13616
E	455	LYS	TYR	engineered mutation	UNP Q13616
G	409	GLY	-	expression tag	UNP Q13616
G	410	SER	-	expression tag	UNP Q13616
G	421	GLU	LEU	engineered mutation	UNP Q13616

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Chain	Residue	Modelled	Actual	Comment	Reference
G	451	GLU	VAL	engineered mutation	UNP Q13616
G	452	LYS	VAL	engineered mutation	UNP Q13616
G	455	LYS	TYR	engineered mutation	UNP Q13616

- Molecule 2 is a protein called E3 ubiquitin-protein ligase RBX1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	86	Total	C	N	O	S	0	0	0
			713	452	129	123	9			
2	D	79	Total	C	N	O	S	0	0	0
			658	419	119	111	9			
2	F	81	Total	C	N	O	S	0	0	0
			684	436	124	115	9			
2	H	81	Total	C	N	O	S	0	0	0
			671	427	121	114	9			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	3	GLY	-	expression tag	UNP P62877
B	4	SER	-	expression tag	UNP P62877
D	3	GLY	-	expression tag	UNP P62877
D	4	SER	-	expression tag	UNP P62877
F	3	GLY	-	expression tag	UNP P62877
F	4	SER	-	expression tag	UNP P62877
H	3	GLY	-	expression tag	UNP P62877
H	4	SER	-	expression tag	UNP P62877

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

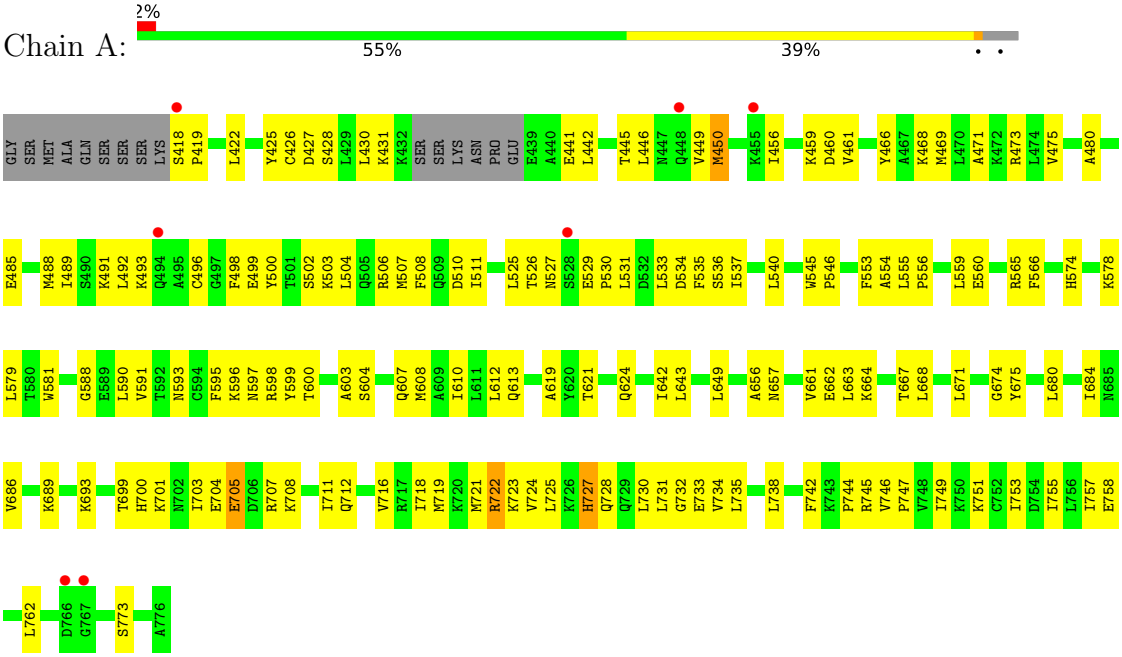
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	3	Total	Zn	0	0
			3	3		
3	D	3	Total	Zn	0	0
			3	3		
3	F	3	Total	Zn	0	0
			3	3		
3	H	3	Total	Zn	0	0
			3	3		

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.

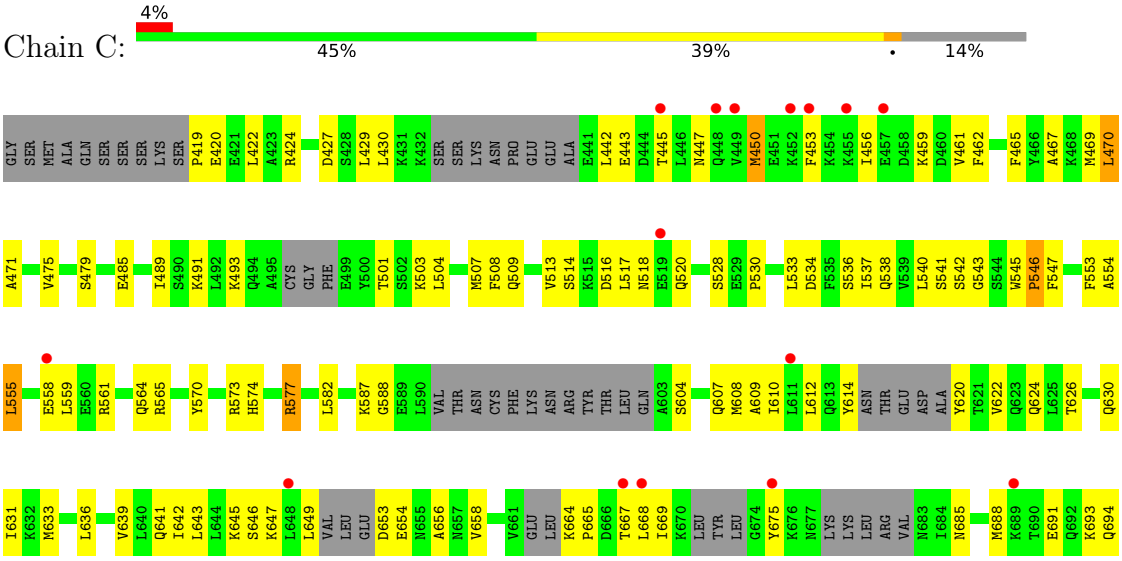
• Molecule 1: Cullin-1

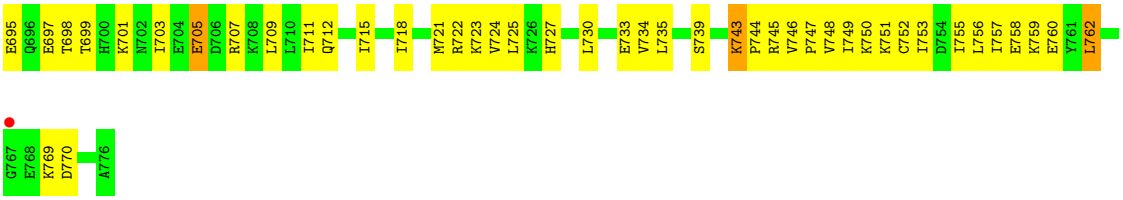
Chain A:



• Molecule 1: Cullin-1

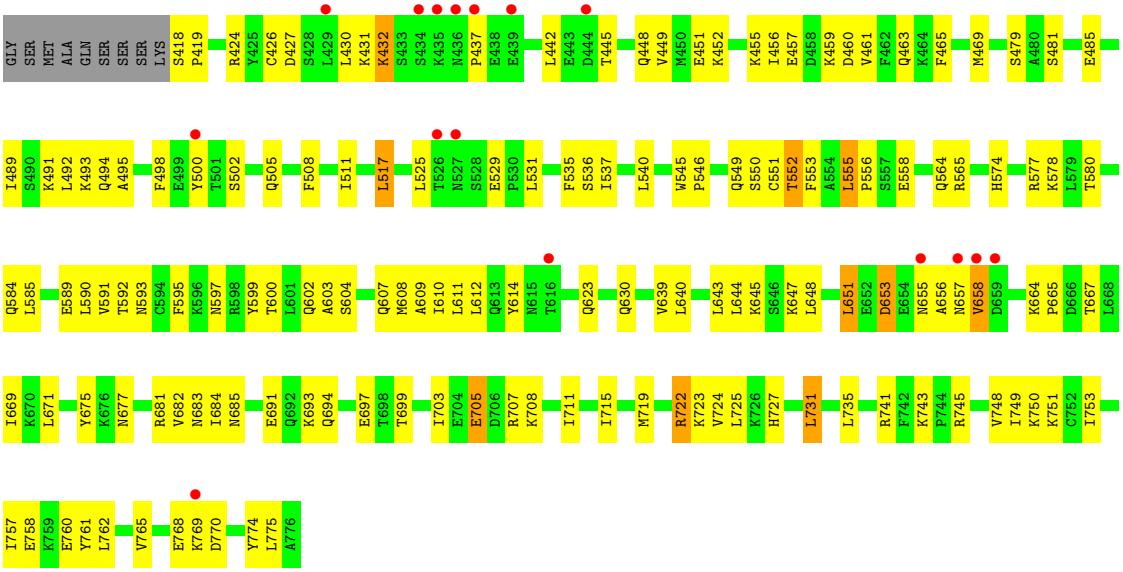
Chain C:





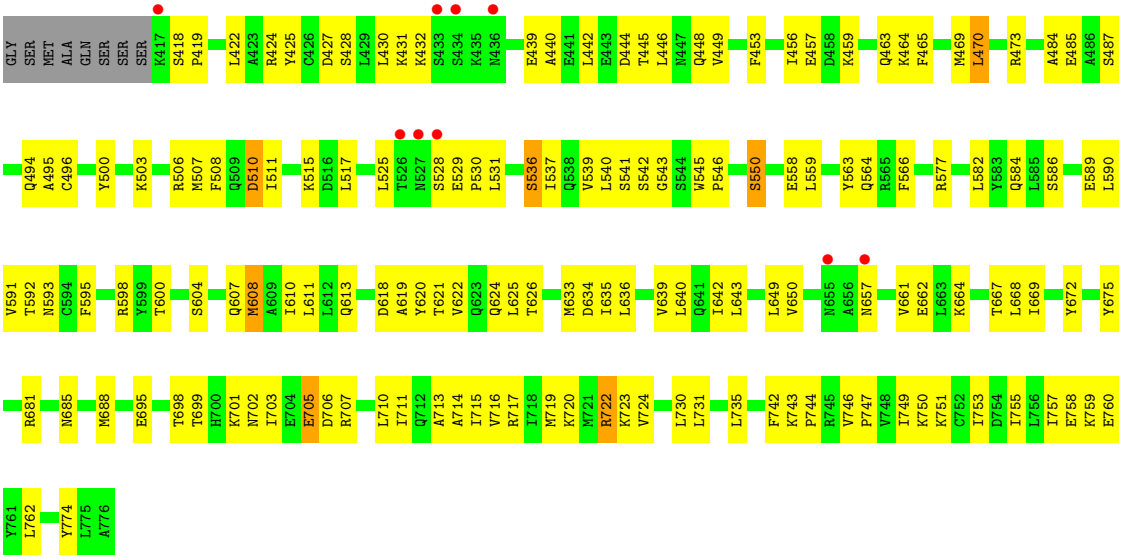
• Molecule 1: Cullin-1

Chain E:



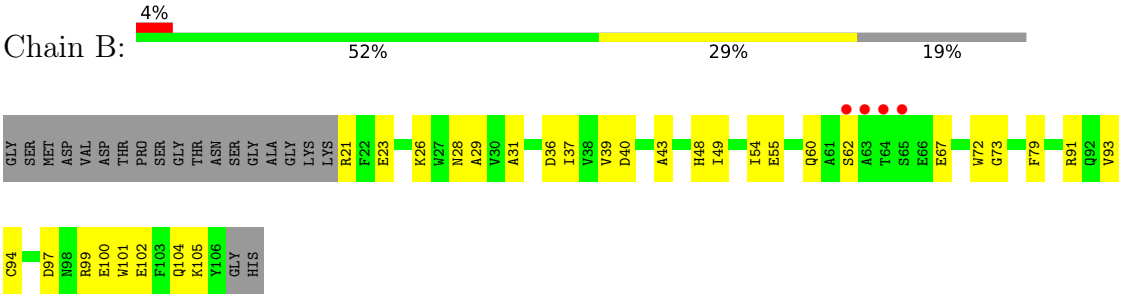
• Molecule 1: Cullin-1

Chain G:



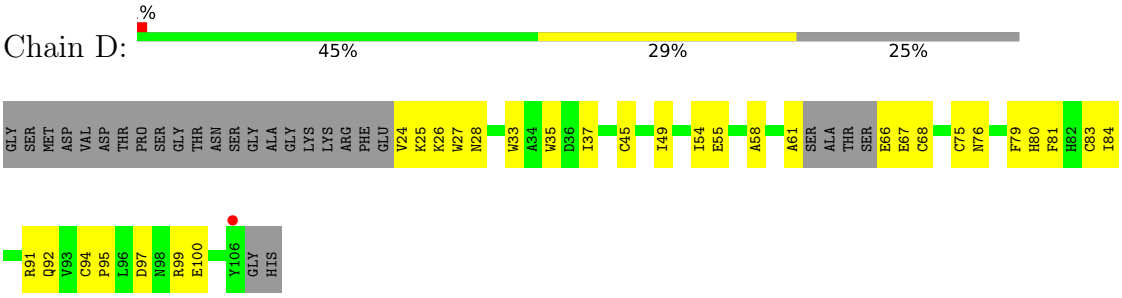
• Molecule 2: E3 ubiquitin-protein ligase RBX1

Chain B:



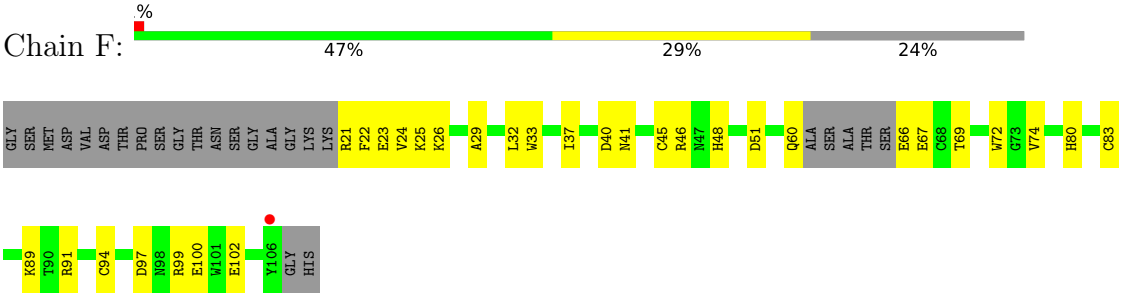
• Molecule 2: E3 ubiquitin-protein ligase RBX1

Chain D:



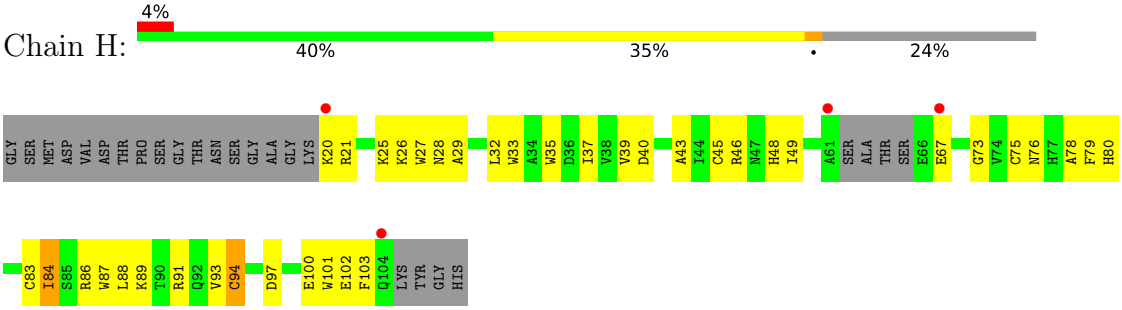
• Molecule 2: E3 ubiquitin-protein ligase RBX1

Chain F:



• Molecule 2: E3 ubiquitin-protein ligase RBX1

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	88.47Å 119.80Å 231.86Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.95 – 3.21 29.95 – 3.21	Depositor EDS
% Data completeness (in resolution range)	99.9 (29.95-3.21) 100.0 (29.95-3.21)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [1]	2.11 (at 3.24Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.5_2)	Depositor
R, R_{free}	0.238 , 0.282 0.232 , 0.280	Depositor DCC
R_{free} test set	2052 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	100.6	Xtriage
Anisotropy	0.177	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 69.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	14055	wwPDB-VP
Average B, all atoms (Å^2)	127.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.10% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.37	0/2911	0.53	0/3910
1	C	0.37	0/2624	0.51	0/3509
1	E	0.36	0/2963	0.50	0/3983
1	G	0.39	0/2982	0.53	0/4006
2	B	0.44	0/734	0.56	0/998
2	D	0.54	1/677 (0.1%)	0.59	0/920
2	F	0.54	1/704 (0.1%)	0.59	0/955
2	H	0.48	0/690	0.55	0/937
All	All	0.40	2/14285 (0.0%)	0.53	0/19218

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	45	CYS	CB-SG	-5.71	1.72	1.81
2	F	45	CYS	CB-SG	-5.35	1.73	1.81

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2870	0	2931	122	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2592	0	2644	138	0
1	E	2918	0	2966	134	0
1	G	2937	0	3001	127	0
2	B	713	0	663	36	0
2	D	658	0	612	30	0
2	F	684	0	635	37	0
2	H	671	0	620	37	0
3	B	3	0	0	0	0
3	D	3	0	0	0	0
3	F	3	0	0	0	0
3	H	3	0	0	0	0
All	All	14055	0	14072	579	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 21.

All (579) 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:E:639:VAL:O	1:E:643:LEU:HD23	1.61	0.98
1:C:743:LYS:HE3	1:C:743:LYS:HA	1.42	0.97
1:A:427:ASP:HB2	1:A:469:MET:HG2	1.43	0.96
1:E:493:LYS:HZ3	1:E:505:GLN:NE2	1.67	0.92
1:E:493:LYS:HZ3	1:E:505:GLN:HE22	1.01	0.92
1:A:718:ILE:HD13	1:A:733:GLU:HB3	1.53	0.90
1:E:705:GLU:OE1	2:F:99:ARG:NH2	2.05	0.90
1:E:647:LYS:H	1:E:647:LYS:HD2	1.36	0.89
1:G:593:ASN:HD22	2:H:21:ARG:HD2	1.37	0.89
1:E:493:LYS:NZ	1:E:505:GLN:HE22	1.72	0.88
1:E:492:LEU:HA	1:E:495:ALA:HB3	1.56	0.88
1:G:525:LEU:HD11	1:G:531:LEU:HG	1.55	0.88
1:C:722:ARG:HD3	1:C:725:LEU:HD13	1.56	0.88
1:E:600:THR:HB	1:E:681:ARG:HG3	1.56	0.88
1:A:701:LYS:O	1:A:705:GLU:HG2	1.73	0.87
1:A:732:GLY:HA2	1:A:735:LEU:HD12	1.57	0.84
1:C:555:LEU:HD11	1:C:559:LEU:HB2	1.58	0.84
1:A:619:ALA:HB1	1:A:668:LEU:HD11	1.61	0.83
1:C:711:ILE:O	1:C:715:ILE:HG13	1.78	0.83
1:E:493:LYS:NZ	1:E:505:GLN:NE2	2.27	0.81
1:A:445:THR:O	1:A:449:VAL:HG23	1.82	0.80
1:G:517:LEU:C	1:G:517:LEU:HD23	2.02	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:492:LEU:O	1:A:496:CYS:HB2	1.81	0.80
1:C:504:LEU:HA	1:C:507:MET:HE2	1.64	0.79
1:A:446:LEU:HG	1:A:488:MET:CE	2.12	0.79
1:A:508:PHE:O	1:A:511:ILE:HG22	1.83	0.79
1:C:703:ILE:O	1:C:707:ARG:HG2	1.83	0.79
1:G:642:ILE:HD11	1:G:688:MET:HB3	1.65	0.79
1:C:701:LYS:O	1:C:705:GLU:HG2	1.84	0.78
1:C:758:GLU:OE2	2:D:92:GLN:N	2.17	0.78
1:E:691:GLU:HA	1:E:694:GLN:NE2	1.97	0.77
1:G:758:GLU:OE1	2:H:91:ARG:HA	1.84	0.77
2:F:37:ILE:HD11	2:H:78:ALA:HB3	1.67	0.76
1:A:442:LEU:O	1:A:446:LEU:HD13	1.85	0.76
2:F:80:HIS:HB2	2:F:83:CYS:SG	2.26	0.76
1:G:463:GLN:HB2	1:G:500:TYR:CZ	2.21	0.76
1:C:517:LEU:O	1:C:517:LEU:HD23	1.86	0.76
1:E:640:LEU:O	1:E:644:LEU:HD13	1.86	0.75
1:A:488:MET:O	1:A:492:LEU:HG	1.88	0.74
1:E:442:LEU:HA	1:E:445:THR:HG22	1.68	0.74
1:G:422:LEU:HD11	1:G:449:VAL:HG13	1.69	0.74
1:G:716:VAL:O	1:G:720:LYS:HB2	1.87	0.74
1:A:758:GLU:OE1	2:B:91:ARG:HA	1.88	0.74
1:C:509:GLN:O	1:C:513:VAL:HG23	1.87	0.74
1:A:642:ILE:HD13	1:A:686:VAL:HG23	1.68	0.74
1:C:758:GLU:HG2	2:D:91:ARG:HG2	1.70	0.73
1:E:705:GLU:OE2	2:F:99:ARG:NH1	2.16	0.73
1:G:742:PHE:O	1:G:744:PRO:HD3	1.88	0.73
2:F:94:CYS:HB3	2:F:97:ASP:OD1	1.89	0.72
1:G:517:LEU:HD23	1:G:517:LEU:O	1.88	0.72
1:E:593:ASN:HB2	2:F:21:ARG:HB3	1.72	0.71
1:C:649:LEU:HD23	1:C:669:ILE:HG21	1.73	0.71
1:A:751:LYS:NZ	2:B:100:GLU:OE1	2.23	0.71
1:G:618:ASP:HB3	2:H:20:LYS:HE3	1.69	0.71
1:G:701:LYS:O	1:G:705:GLU:HG3	1.90	0.71
1:A:461:VAL:HA	1:A:703:ILE:HD13	1.71	0.71
1:E:465:PHE:O	1:E:469:MET:HG2	1.89	0.71
1:C:693:LYS:O	1:C:697:GLU:HG3	1.90	0.71
1:C:607:GLN:HG2	1:C:643:LEU:HD21	1.72	0.70
1:G:657:ASN:HB3	1:G:661:VAL:HG23	1.73	0.70
1:A:746:VAL:N	1:A:747:PRO:HD2	2.07	0.70
2:B:40:ASP:OD1	2:B:48:HIS:NE2	2.25	0.70
1:C:751:LYS:NZ	2:D:100:GLU:OE2	2.24	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:558:GLU:HG3	1:C:612:LEU:HD13	1.73	0.69
1:G:757:ILE:HG12	1:G:762:LEU:HD12	1.75	0.69
1:A:460:ASP:OD2	1:A:707:ARG:HD3	1.93	0.68
1:G:604:SER:HB3	1:G:685:ASN:OD1	1.94	0.68
1:A:664:LYS:HB2	1:A:667:THR:HG23	1.73	0.68
1:C:758:GLU:OE2	2:D:91:ARG:HA	1.93	0.68
1:C:709:LEU:HD23	1:C:712:GLN:OE1	1.92	0.68
2:B:94:CYS:HB3	2:B:97:ASP:OD1	1.94	0.67
1:E:442:LEU:O	1:E:445:THR:HG22	1.93	0.67
1:G:427:ASP:HB2	1:G:469:MET:HG2	1.76	0.67
1:G:445:THR:O	1:G:449:VAL:HG23	1.95	0.67
1:E:595:PHE:CD2	1:E:675:TYR:HB3	2.30	0.67
1:C:489:ILE:HD11	1:C:508:PHE:CZ	2.29	0.67
1:C:641:GLN:O	1:C:645:LYS:HD3	1.95	0.67
1:E:760:GLU:O	1:E:775:LEU:HD12	1.94	0.66
1:G:710:LEU:HD13	1:G:742:PHE:HE2	1.61	0.66
1:G:715:ILE:HD13	1:G:753:ILE:HG12	1.76	0.66
1:A:471:ALA:O	1:A:475:VAL:HG23	1.95	0.66
1:A:701:LYS:O	1:A:705:GLU:CG	2.44	0.66
1:E:445:THR:O	1:E:449:VAL:HG23	1.95	0.66
1:C:757:ILE:HG12	1:C:762:LEU:HD12	1.77	0.66
1:G:751:LYS:NZ	2:H:100:GLU:OE1	2.28	0.66
2:D:61:ALA:HB1	2:D:66:GLU:HG3	1.78	0.66
1:E:494:GLN:O	1:E:494:GLN:HG2	1.96	0.65
1:G:701:LYS:O	1:G:705:GLU:CG	2.44	0.65
1:A:724:VAL:HG22	1:A:773:SER:HB2	1.78	0.65
1:C:588:GLY:HA3	1:C:608:MET:SD	2.37	0.65
1:C:750:LYS:HD2	1:C:750:LYS:O	1.97	0.65
1:E:456:ILE:O	1:E:459:LYS:HE2	1.96	0.65
1:A:526:THR:O	1:A:527:ASN:OD1	2.15	0.65
1:A:663:LEU:HD12	1:A:663:LEU:H	1.61	0.65
2:H:88:LEU:HD11	2:H:101:TRP:CD1	2.32	0.64
1:A:556:PRO:HD2	1:A:559:LEU:HD12	1.79	0.64
1:E:743:LYS:HE3	1:E:743:LYS:HA	1.77	0.64
2:H:94:CYS:HB3	2:H:97:ASP:OD1	1.97	0.64
1:C:520:GLN:HA	1:C:520:GLN:OE1	1.98	0.64
1:C:540:LEU:HD13	1:C:545:TRP:CD2	2.33	0.64
1:G:699:THR:O	1:G:703:ILE:HG13	1.98	0.63
1:A:578:LYS:HB3	2:B:36:ASP:HB2	1.79	0.63
1:G:626:THR:OG1	1:G:633:MET:HG2	1.98	0.63
1:A:590:LEU:HD11	1:A:608:MET:HA	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:705:GLU:OE2	2:B:99:ARG:NH1	2.32	0.63
1:C:427:ASP:HB2	1:C:469:MET:HG2	1.81	0.63
1:A:708:LYS:NZ	1:A:751:LYS:HD3	2.13	0.63
2:B:37:ILE:HG22	2:B:39:VAL:HG23	1.81	0.63
2:H:37:ILE:HG22	2:H:39:VAL:HG23	1.81	0.63
1:E:719:MET:HB3	1:E:774:TYR:HB2	1.81	0.62
1:G:650:VAL:HG22	1:G:672:TYR:HB2	1.82	0.62
1:E:647:LYS:HD2	1:E:647:LYS:N	2.13	0.62
1:G:600:THR:HB	1:G:681:ARG:HG3	1.80	0.62
2:F:40:ASP:HB3	2:F:48:HIS:CD2	2.34	0.62
1:A:426:CYS:O	1:A:430:LEU:HD13	2.00	0.62
1:A:744:PRO:HB2	1:A:749:ILE:HD11	1.82	0.61
1:A:579:LEU:HD22	2:B:31:ALA:HB1	1.81	0.61
1:A:597:ASN:HB2	1:A:599:TYR:CE1	2.34	0.61
1:A:746:VAL:N	1:A:747:PRO:CD	2.63	0.61
1:G:714:ALA:HA	1:G:717:ARG:NH1	2.15	0.61
1:A:591:VAL:CG1	2:B:23:GLU:HB2	2.31	0.61
1:C:703:ILE:O	1:C:707:ARG:CG	2.49	0.61
1:G:425:TYR:O	1:G:428:SER:HB3	1.99	0.61
1:G:540:LEU:HB3	1:G:545:TRP:CD1	2.36	0.61
1:A:722:ARG:HD3	1:A:725:LEU:HD13	1.82	0.61
1:C:467:ALA:HB2	1:C:504:LEU:HD21	1.83	0.60
1:C:769:LYS:HG3	1:C:770:ASP:H	1.67	0.60
1:G:577:ARG:HD3	2:H:33:TRP:CE3	2.36	0.60
1:G:591:VAL:HG11	2:H:25:LYS:HE3	1.83	0.60
2:H:84:ILE:HG13	2:H:84:ILE:O	2.02	0.60
1:C:471:ALA:O	1:C:475:VAL:HG23	2.02	0.60
1:E:602:GLN:HB2	1:E:683:ASN:HD22	1.67	0.60
1:C:705:GLU:OE1	2:D:99:ARG:NH1	2.30	0.60
1:G:714:ALA:HA	1:G:717:ARG:HH12	1.66	0.60
1:E:769:LYS:HG3	1:E:770:ASP:H	1.67	0.60
1:G:633:MET:HA	1:G:636:LEU:HB3	1.83	0.60
1:A:450:MET:HG3	1:A:491:LYS:HB3	1.83	0.59
1:C:753:ILE:O	1:C:757:ILE:HG13	2.02	0.59
1:E:691:GLU:O	1:E:694:GLN:HG2	2.02	0.59
1:G:707:ARG:O	1:G:711:ILE:HG13	2.02	0.59
1:E:607:GLN:HE22	1:E:685:ASN:HA	1.68	0.59
1:G:593:ASN:HD22	2:H:21:ARG:CD	2.12	0.59
1:E:578:LYS:O	2:F:33:TRP:HA	2.02	0.59
2:B:104:GLN:HG3	2:B:105:LYS:HG2	1.84	0.59
1:E:517:LEU:O	1:E:517:LEU:HD23	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:661:VAL:HG12	1:G:661:VAL:O	2.02	0.59
1:A:507:MET:HB3	1:A:545:TRP:CH2	2.38	0.59
1:A:597:ASN:HB2	1:A:599:TYR:CZ	2.38	0.58
1:C:642:ILE:HD11	1:C:688:MET:HB3	1.85	0.58
1:C:718:ILE:HD13	1:C:733:GLU:HB3	1.85	0.58
1:E:525:LEU:HD21	1:E:531:LEU:HD12	1.85	0.58
2:B:40:ASP:OD1	2:B:48:HIS:CD2	2.56	0.58
1:C:419:PRO:HB3	1:C:456:ILE:HG21	1.84	0.58
1:C:610:ILE:HD11	1:C:643:LEU:HG	1.85	0.58
1:E:597:ASN:HB2	1:E:599:TYR:CE1	2.39	0.58
1:G:508:PHE:O	1:G:511:ILE:HG22	2.04	0.58
1:A:607:GLN:HG2	1:A:643:LEU:HD21	1.85	0.58
1:C:453:PHE:CE1	1:C:462:PHE:CD2	2.91	0.58
1:A:708:LYS:HZ2	1:A:751:LYS:HD3	1.69	0.58
1:C:528:SER:O	1:C:530:PRO:HD3	2.02	0.58
2:D:94:CYS:HB3	2:D:97:ASP:OD1	2.03	0.58
1:G:503:LYS:O	1:G:507:MET:HG3	2.03	0.58
1:G:430:LEU:HD11	1:G:446:LEU:HD21	1.85	0.58
1:A:540:LEU:HB3	1:A:545:TRP:NE1	2.19	0.58
1:A:536:SER:O	2:B:28:ASN:HA	2.04	0.57
1:A:485:GLU:HB3	1:A:508:PHE:HZ	1.69	0.57
1:E:508:PHE:O	1:E:511:ILE:HG22	2.05	0.57
1:A:593:ASN:HB2	2:B:21:ARG:HD2	1.86	0.57
1:A:703:ILE:O	1:A:707:ARG:HG3	2.05	0.57
1:C:614:TYR:CE1	1:C:620:TYR:HD1	2.22	0.57
2:H:93:VAL:O	2:H:93:VAL:HG23	2.05	0.57
1:A:722:ARG:NH1	1:A:733:GLU:OE2	2.38	0.57
1:E:758:GLU:OE1	2:F:91:ARG:HA	2.05	0.57
1:C:620:TYR:HA	1:C:624:GLN:OE1	2.04	0.57
2:B:49:ILE:HD12	2:D:35:TRP:HB2	1.87	0.57
1:A:588:GLY:HA3	1:A:608:MET:SD	2.45	0.56
1:A:603:ALA:HB2	1:A:684:ILE:HD11	1.87	0.56
1:C:699:THR:O	1:C:703:ILE:HG13	2.04	0.56
2:B:49:ILE:HD13	2:D:37:ILE:HD11	1.86	0.56
2:F:67:GLU:O	2:F:69:THR:HG23	2.06	0.56
1:A:712:GLN:O	1:A:716:VAL:HG23	2.06	0.56
1:G:620:TYR:HB2	1:G:625:LEU:CD1	2.36	0.56
1:A:596:LYS:HE2	1:A:674:GLY:HA2	1.87	0.56
2:D:25:LYS:HE3	2:D:25:LYS:HA	1.88	0.56
1:C:504:LEU:O	1:C:508:PHE:CD1	2.59	0.55
1:A:485:GLU:O	1:A:489:ILE:HG13	2.05	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:751:LYS:CE	2:F:100:GLU:OE1	2.54	0.55
1:C:691:GLU:O	1:C:694:GLN:HG2	2.06	0.55
1:E:724:VAL:HG12	1:E:725:LEU:N	2.21	0.55
1:G:755:ILE:HG22	1:G:759:LYS:HD2	1.87	0.55
1:A:730:LEU:O	1:A:734:VAL:HG23	2.06	0.55
1:C:489:ILE:O	1:C:493:LYS:HB2	2.06	0.55
1:G:592:THR:O	1:G:598:ARG:HD2	2.06	0.55
1:A:656:ALA:HB1	1:A:661:VAL:HG21	1.87	0.55
1:C:518:ASN:HD21	1:C:536:SER:HA	1.72	0.55
1:C:514:SER:OG	1:C:538:GLN:HA	2.06	0.55
1:C:722:ARG:HD3	1:C:725:LEU:CD1	2.31	0.55
1:G:444:ASP:O	1:G:448:GLN:HG3	2.06	0.55
1:E:537:ILE:HA	2:F:29:ALA:O	2.07	0.55
1:E:657:ASN:O	1:E:658:VAL:HB	2.07	0.55
1:E:418:SER:HB3	1:E:419:PRO:HD3	1.89	0.54
2:D:81:PHE:CE2	2:F:89:LYS:HD2	2.41	0.54
1:G:465:PHE:O	1:G:469:MET:HB2	2.07	0.54
1:A:749:ILE:O	1:A:753:ILE:HG13	2.08	0.54
1:C:533:LEU:HD22	2:D:24:VAL:HG11	1.89	0.54
1:E:608:MET:O	1:E:612:LEU:HD23	2.07	0.54
1:G:529:GLU:HG3	1:G:530:PRO:N	2.23	0.54
1:A:579:LEU:HD22	2:B:31:ALA:CB	2.38	0.54
1:C:570:TYR:CE1	1:C:574:HIS:CD2	2.96	0.54
1:C:653:ASP:OD2	1:C:656:ALA:HB2	2.07	0.54
1:E:751:LYS:NZ	2:F:100:GLU:OE1	2.39	0.54
1:A:419:PRO:HA	1:A:422:LEU:HD12	1.89	0.53
1:E:705:GLU:CD	2:F:99:ARG:HH12	2.08	0.53
1:G:540:LEU:HB3	1:G:545:TRP:NE1	2.23	0.53
1:E:651:LEU:HD12	1:E:651:LEU:H	1.73	0.53
1:A:705:GLU:OE1	2:B:99:ARG:NH2	2.41	0.53
2:B:37:ILE:HG22	2:B:39:VAL:CG2	2.39	0.53
1:C:752:CYS:O	1:C:756:LEU:HG	2.09	0.53
1:E:647:LYS:H	1:E:647:LYS:CD	2.09	0.53
2:H:87:TRP:HH2	2:H:93:VAL:O	1.92	0.53
2:H:88:LEU:HD11	2:H:101:TRP:HD1	1.73	0.53
1:E:437:PRO:HD2	1:E:442:LEU:HD11	1.91	0.53
2:F:60:GLN:OE1	2:F:60:GLN:HA	2.08	0.53
2:F:72:TRP:CH2	2:H:35:TRP:HB3	2.43	0.53
1:C:577:ARG:HD2	2:D:33:TRP:CE3	2.43	0.53
1:G:517:LEU:C	1:G:517:LEU:CD2	2.72	0.53
1:C:701:LYS:O	1:C:705:GLU:CG	2.54	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:755:ILE:HG22	1:C:759:LYS:HD2	1.90	0.53
1:E:500:TYR:OH	1:E:741:ARG:NE	2.42	0.53
1:E:591:VAL:HG13	2:F:23:GLU:HB2	1.91	0.53
1:G:529:GLU:CD	1:G:530:PRO:HD2	2.30	0.53
2:D:67:GLU:O	2:D:67:GLU:HG2	2.07	0.53
1:E:424:ARG:CG	1:E:469:MET:HE1	2.39	0.53
1:A:441:GLU:HG3	1:A:442:LEU:HD12	1.91	0.52
1:E:751:LYS:HE3	2:F:100:GLU:OE1	2.08	0.52
1:G:607:GLN:HG2	1:G:643:LEU:HD21	1.91	0.52
1:C:749:ILE:O	1:C:753:ILE:HG13	2.09	0.52
1:E:614:TYR:OH	1:E:669:ILE:HG22	2.09	0.52
1:G:619:ALA:HA	1:G:669:ILE:O	2.09	0.52
1:A:525:LEU:HD21	1:A:531:LEU:HD12	1.92	0.52
1:G:424:ARG:HG2	1:G:469:MET:HE3	1.91	0.52
1:E:623:GLN:HB2	1:E:665:PRO:HB3	1.91	0.52
1:E:647:LYS:O	1:E:675:TYR:CD2	2.62	0.52
1:A:537:ILE:HG13	2:B:29:ALA:HB3	1.91	0.52
1:A:540:LEU:HB3	1:A:545:TRP:CD1	2.45	0.52
1:A:727:HIS:NE2	1:A:731:LEU:HD21	2.24	0.52
1:G:470:LEU:HD11	1:G:508:PHE:HE1	1.74	0.52
1:A:425:TYR:O	1:A:428:SER:HB3	2.09	0.52
1:G:749:ILE:O	1:G:753:ILE:HG13	2.10	0.52
1:A:604:SER:O	1:A:608:MET:HG3	2.10	0.52
1:G:453:PHE:HA	1:G:456:ILE:HG12	1.92	0.52
1:G:758:GLU:O	2:H:91:ARG:NH1	2.42	0.52
1:A:534:ASP:HB3	2:B:26:LYS:HG2	1.92	0.52
1:E:722:ARG:O	1:E:724:VAL:N	2.43	0.52
1:C:447:ASN:HA	1:C:450:MET:HB2	1.92	0.52
1:A:745:ARG:C	1:A:747:PRO:HD2	2.30	0.52
1:C:758:GLU:CG	2:D:91:ARG:HG2	2.37	0.52
1:G:755:ILE:HG23	2:H:93:VAL:HG21	1.91	0.52
1:E:564:GLN:HE22	1:G:564:GLN:NE2	2.08	0.51
1:G:525:LEU:HD11	1:G:531:LEU:CG	2.34	0.51
1:G:743:LYS:HE3	1:G:743:LYS:HA	1.92	0.51
2:D:55:GLU:O	2:D:58:ALA:HB3	2.11	0.51
1:C:422:LEU:HG	1:C:462:PHE:CE1	2.45	0.51
1:E:711:ILE:O	1:E:715:ILE:HG13	2.10	0.51
2:H:73:GLY:HA2	2:H:102:GLU:O	2.11	0.51
1:C:461:VAL:O	1:C:465:PHE:HD1	1.93	0.51
1:C:633:MET:HA	1:C:636:LEU:HB3	1.93	0.51
1:E:691:GLU:HA	1:E:694:GLN:CD	2.29	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:540:LEU:HB3	1:E:545:TRP:NE1	2.26	0.51
1:C:554:ALA:HB2	1:C:630:GLN:CG	2.41	0.51
1:G:439:GLU:HG3	1:G:440:ALA:H	1.76	0.51
1:E:591:VAL:HG11	2:F:25:LYS:HE3	1.91	0.51
2:B:73:GLY:HA2	2:B:102:GLU:O	2.10	0.51
1:G:695:GLU:O	1:G:698:THR:HG22	2.10	0.51
1:A:418:SER:HB3	1:A:419:PRO:HD3	1.94	0.50
2:F:66:GLU:HG2	2:F:67:GLU:N	2.26	0.50
1:C:559:LEU:HD22	2:D:27:TRP:CD2	2.46	0.50
1:E:442:LEU:CA	1:E:445:THR:HG22	2.37	0.50
1:C:649:LEU:HD23	1:C:669:ILE:CG2	2.40	0.50
1:G:621:THR:OG1	1:G:624:GLN:HG3	2.12	0.50
1:G:719:MET:HE2	1:G:730:LEU:HD13	1.93	0.50
2:B:54:ILE:HG23	2:B:55:GLU:N	2.27	0.50
1:C:516:ASP:OD1	1:C:516:ASP:C	2.49	0.50
1:C:536:SER:O	2:D:28:ASN:HA	2.11	0.50
1:C:744:PRO:HB2	1:C:749:ILE:HD11	1.93	0.50
1:E:574:HIS:HB2	1:E:577:ARG:HG3	1.92	0.50
1:C:553:PHE:HZ	1:C:609:ALA:HB2	1.76	0.50
1:C:755:ILE:O	1:C:759:LYS:HG3	2.12	0.50
1:E:593:ASN:HD22	2:F:21:ARG:HG2	1.77	0.50
1:G:457:GLU:N	1:G:457:GLU:OE2	2.45	0.50
1:A:489:ILE:HD11	1:A:508:PHE:CE1	2.47	0.49
1:C:443:GLU:OE1	1:C:491:LYS:HE3	2.12	0.49
1:A:460:ASP:OD1	1:A:461:VAL:N	2.45	0.49
1:C:554:ALA:HB2	1:C:630:GLN:HB2	1.94	0.49
1:E:432:LYS:HE3	1:E:479:SER:O	2.13	0.49
1:E:549:GLN:HG3	1:E:550:SER:O	2.11	0.49
1:A:529:GLU:HB3	1:A:565:ARG:NH1	2.27	0.49
1:E:485:GLU:O	1:E:489:ILE:HG13	2.13	0.49
1:G:755:ILE:O	1:G:759:LYS:HG3	2.11	0.49
2:H:80:HIS:HB2	2:H:83:CYS:SG	2.53	0.49
1:C:534:ASP:HB3	2:D:26:LYS:HG2	1.95	0.49
1:G:418:SER:HB3	1:G:419:PRO:HD3	1.94	0.49
1:C:420:GLU:OE2	1:C:424:ARG:HD2	2.13	0.49
1:C:517:LEU:HD23	1:C:517:LEU:C	2.32	0.49
1:E:461:VAL:HA	1:E:703:ILE:HD13	1.94	0.49
1:E:481:SER:O	1:E:485:GLU:HG2	2.12	0.49
1:E:608:MET:CE	2:F:24:VAL:HG13	2.42	0.49
1:A:504:LEU:HA	1:A:507:MET:HE2	1.95	0.49
1:C:587:LYS:O	2:D:27:TRP:CD1	2.65	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:72:TRP:CZ2	2:H:35:TRP:HB3	2.48	0.49
1:C:647:LYS:O	1:C:675:TYR:HD2	1.95	0.49
1:G:453:PHE:O	1:G:459:LYS:HE2	2.13	0.48
1:C:759:LYS:O	1:C:760:GLU:HB2	2.13	0.48
1:E:591:VAL:CG1	2:F:23:GLU:HB2	2.43	0.48
1:E:727:HIS:NE2	1:E:731:LEU:HD12	2.28	0.48
1:G:619:ALA:HB1	1:G:668:LEU:HD11	1.95	0.48
2:H:86:ARG:HA	2:H:89:LYS:HD3	1.95	0.48
1:G:453:PHE:CE1	1:G:459:LYS:HD2	2.48	0.48
1:G:550:SER:HA	1:G:584:GLN:OE1	2.13	0.48
1:A:446:LEU:HG	1:A:488:MET:HE1	1.91	0.48
1:C:746:VAL:N	1:C:747:PRO:CD	2.76	0.48
1:E:457:GLU:N	1:E:457:GLU:OE2	2.47	0.48
1:C:642:ILE:HD11	1:C:688:MET:HA	1.95	0.48
1:E:603:ALA:HB2	1:E:684:ILE:HD11	1.95	0.48
1:A:537:ILE:HD13	1:A:566:PHE:CE2	2.49	0.48
1:A:722:ARG:O	1:A:724:VAL:N	2.47	0.48
1:C:758:GLU:OE2	2:D:91:ARG:CA	2.62	0.48
1:E:564:GLN:HE22	1:G:564:GLN:HE22	1.61	0.48
1:E:675:TYR:CZ	1:E:677:ASN:HB2	2.49	0.48
2:B:91:ARG:NH2	1:C:760:GLU:OE2	2.47	0.47
1:A:738:LEU:HD23	1:A:742:PHE:CZ	2.49	0.47
1:C:419:PRO:HG3	1:C:456:ILE:HD12	1.96	0.47
1:C:461:VAL:HA	1:C:703:ILE:HD13	1.95	0.47
1:C:504:LEU:O	1:C:508:PHE:HD1	1.96	0.47
1:G:473:ARG:NH1	1:G:485:GLU:OE2	2.45	0.47
1:A:427:ASP:HB2	1:A:469:MET:CG	2.29	0.47
1:C:707:ARG:O	1:C:711:ILE:HG13	2.14	0.47
1:A:728:GLN:O	1:A:731:LEU:HB2	2.14	0.47
1:E:693:LYS:N	1:E:693:LYS:HD2	2.30	0.47
1:E:644:LEU:HB3	1:E:658:VAL:HG13	1.96	0.47
1:E:745:ARG:O	1:E:749:ILE:HG13	2.15	0.47
1:A:742:PHE:O	1:A:744:PRO:HD3	2.15	0.47
1:C:429:LEU:HB2	1:C:430:LEU:HD12	1.96	0.47
1:C:604:SER:HB3	1:C:685:ASN:OD1	2.14	0.47
1:C:722:ARG:CD	1:C:725:LEU:HD13	2.38	0.47
1:G:610:ILE:HD11	1:G:643:LEU:HG	1.96	0.47
1:A:489:ILE:O	1:A:493:LYS:HB2	2.15	0.47
1:A:727:HIS:CD2	1:A:731:LEU:HD23	2.50	0.47
1:G:751:LYS:O	1:G:755:ILE:HG13	2.15	0.47
1:C:430:LEU:HD12	1:C:430:LEU:N	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:501:THR:HA	1:C:504:LEU:HD12	1.96	0.46
1:G:442:LEU:HA	1:G:445:THR:OG1	2.15	0.46
1:C:553:PHE:CZ	1:C:609:ALA:HB2	2.49	0.46
1:A:525:LEU:HD11	1:A:531:LEU:HG	1.96	0.46
1:A:595:PHE:CD2	1:A:675:TYR:HB3	2.50	0.46
2:B:67:GLU:HA	2:B:67:GLU:OE1	2.15	0.46
1:E:769:LYS:HG3	1:E:770:ASP:N	2.30	0.46
1:G:586:SER:OG	2:H:29:ALA:HA	2.14	0.46
1:C:695:GLU:O	1:C:698:THR:HG22	2.16	0.46
1:E:442:LEU:HA	1:E:445:THR:CG2	2.40	0.46
1:E:540:LEU:O	2:F:32:LEU:HA	2.16	0.46
1:E:553:PHE:CZ	1:E:609:ALA:HB2	2.50	0.46
1:G:419:PRO:HG3	1:G:456:ILE:HG23	1.97	0.46
1:C:730:LEU:O	1:C:734:VAL:HG23	2.15	0.46
1:G:604:SER:O	1:G:608:MET:HG3	2.16	0.46
1:G:730:LEU:HD23	1:G:753:ILE:HD13	1.98	0.46
1:A:608:MET:O	1:A:612:LEU:HG	2.15	0.46
1:E:491:LYS:O	1:E:495:ALA:HB2	2.16	0.46
1:G:470:LEU:HD23	1:G:470:LEU:O	2.16	0.46
1:G:701:LYS:O	1:G:705:GLU:HG2	2.15	0.46
1:A:533:LEU:CD1	1:A:535:PHE:HB2	2.45	0.46
1:E:653:ASP:C	1:E:655:ASN:H	2.19	0.46
1:A:427:ASP:O	1:A:431:LYS:HB2	2.16	0.46
1:C:668:LEU:O	1:C:669:ILE:HD13	2.16	0.46
1:E:648:LEU:O	1:E:671:LEU:HD22	2.16	0.46
1:E:658:VAL:HG12	1:E:658:VAL:O	2.16	0.46
1:G:506:ARG:O	1:G:510:ASP:HB2	2.16	0.46
1:G:531:LEU:HD23	1:G:531:LEU:HA	1.78	0.46
1:G:539:VAL:O	1:G:540:LEU:HD23	2.16	0.46
2:D:75:CYS:O	2:D:76:ASN:HB2	2.16	0.45
1:G:541:SER:O	1:G:543:GLY:N	2.49	0.45
1:G:722:ARG:O	1:G:724:VAL:N	2.50	0.45
1:G:759:LYS:O	1:G:760:GLU:HB2	2.16	0.45
2:H:75:CYS:O	2:H:76:ASN:HB2	2.15	0.45
1:A:427:ASP:CB	1:A:469:MET:HG2	2.31	0.45
1:A:503:LYS:O	1:A:507:MET:HG3	2.16	0.45
2:B:43:ALA:HB3	2:B:79:PHE:HE2	1.81	0.45
1:E:664:LYS:HB2	1:E:667:THR:HG23	1.97	0.45
1:E:677:ASN:OD1	1:E:682:VAL:HG22	2.16	0.45
1:E:703:ILE:O	1:E:707:ARG:HG3	2.16	0.45
1:G:640:LEU:HA	1:G:640:LEU:HD23	1.79	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:87:TRP:CE2	2:H:91:ARG:HD2	2.51	0.45
1:A:610:ILE:O	1:A:613:GLN:HB2	2.16	0.45
1:A:758:GLU:O	2:B:91:ARG:NH1	2.49	0.45
2:D:80:HIS:HB2	2:D:83:CYS:SG	2.57	0.45
1:E:731:LEU:O	1:E:735:LEU:HG	2.16	0.45
1:C:442:LEU:HA	1:C:445:THR:HG22	1.99	0.45
1:G:559:LEU:HD22	2:H:27:TRP:CD2	2.51	0.45
1:G:747:PRO:O	1:G:750:LYS:HB3	2.16	0.45
1:A:719:MET:CE	1:A:719:MET:HA	2.46	0.45
1:C:453:PHE:O	1:C:459:LYS:HE2	2.17	0.45
1:C:626:THR:O	1:C:626:THR:HG22	2.16	0.45
2:B:104:GLN:HG3	2:B:105:LYS:N	2.32	0.45
1:C:727:HIS:C	1:C:727:HIS:CD2	2.90	0.45
1:G:590:LEU:HD12	1:G:611:LEU:HD12	1.99	0.45
1:E:765:VAL:O	1:E:768:GLU:HB2	2.16	0.45
1:C:722:ARG:O	1:C:724:VAL:N	2.50	0.45
1:E:456:ILE:HG22	1:E:457:GLU:N	2.32	0.45
1:G:545:TRP:HA	1:G:546:PRO:HD3	1.84	0.45
1:A:499:GLU:HA	1:A:502:SER:HB2	1.98	0.45
1:A:700:HIS:O	1:A:704:GLU:HG2	2.17	0.45
1:A:731:LEU:O	1:A:735:LEU:HG	2.17	0.45
1:C:489:ILE:CD1	1:C:508:PHE:CZ	3.00	0.45
1:C:745:ARG:HB2	1:C:748:VAL:HG23	1.98	0.45
1:G:536:SER:O	2:H:28:ASN:HA	2.17	0.45
1:A:493:LYS:HE3	1:A:498:PHE:CD1	2.52	0.44
1:C:503:LYS:O	1:C:507:MET:HG3	2.17	0.44
1:E:448:GLN:O	1:E:452:LYS:HG3	2.17	0.44
1:E:549:GLN:OE1	1:E:580:THR:HG23	2.17	0.44
1:G:537:ILE:HD13	1:G:566:PHE:CE2	2.53	0.44
1:A:529:GLU:HA	1:A:530:PRO:HD3	1.86	0.44
1:C:420:GLU:HG2	1:C:424:ARG:HD3	2.00	0.44
1:E:584:GLN:HG2	1:E:585:LEU:HG	1.98	0.44
2:F:40:ASP:HB3	2:F:48:HIS:HD2	1.80	0.44
1:G:582:LEU:HD11	2:H:32:LEU:HG	1.99	0.44
1:G:620:TYR:HB3	1:G:624:GLN:HB2	1.99	0.44
2:D:49:ILE:HG22	2:D:49:ILE:O	2.17	0.44
1:E:498:PHE:O	1:E:502:SER:HB2	2.17	0.44
1:G:427:ASP:O	1:G:431:LYS:HB2	2.17	0.44
1:G:595:PHE:CD2	1:G:675:TYR:HB3	2.53	0.44
1:G:664:LYS:HB2	1:G:667:THR:HG23	1.99	0.44
1:G:719:MET:HB3	1:G:774:TYR:HB2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:719:MET:CE	1:G:730:LEU:HD13	2.46	0.44
1:C:573:ARG:HD2	1:C:573:ARG:O	2.17	0.44
1:C:664:LYS:HB2	1:C:667:THR:HG23	1.99	0.44
1:E:427:ASP:O	1:E:431:LYS:HB2	2.18	0.44
1:A:506:ARG:O	1:A:510:ASP:HB2	2.18	0.44
1:C:626:THR:OG1	1:C:633:MET:HG2	2.18	0.44
1:E:424:ARG:HG3	1:E:469:MET:HE1	2.00	0.44
1:G:432:LYS:HG3	1:G:432:LYS:O	2.18	0.44
1:A:468:LYS:HD3	1:A:699:THR:OG1	2.18	0.44
1:A:545:TRP:HA	1:A:546:PRO:HD3	1.80	0.44
2:D:54:ILE:HG23	2:D:55:GLU:N	2.33	0.44
1:E:648:LEU:HD11	1:E:684:ILE:HG21	1.99	0.44
2:F:37:ILE:HD12	2:H:78:ALA:H	1.83	0.44
1:G:607:GLN:O	1:G:608:MET:C	2.55	0.44
1:A:758:GLU:OE2	2:B:93:VAL:HG22	2.18	0.44
1:C:541:SER:C	1:C:543:GLY:H	2.22	0.44
1:C:735:LEU:O	1:C:739:SER:HB2	2.17	0.44
1:E:437:PRO:HB2	1:E:442:LEU:HD12	1.98	0.44
1:E:699:THR:O	1:E:703:ILE:HG13	2.18	0.44
1:E:708:LYS:HE3	1:E:748:VAL:HG13	2.00	0.44
1:E:691:GLU:HA	1:E:694:GLN:HE21	1.82	0.43
1:G:558:GLU:CD	1:G:558:GLU:H	2.20	0.43
1:A:657:ASN:O	1:A:661:VAL:HG23	2.17	0.43
1:A:705:GLU:HG2	1:A:705:GLU:H	1.50	0.43
1:C:757:ILE:HG12	1:C:762:LEU:CD1	2.46	0.43
1:E:545:TRP:HA	1:E:546:PRO:HD3	1.69	0.43
1:E:757:ILE:HG12	1:E:762:LEU:HD12	2.01	0.43
1:A:757:ILE:HG12	1:A:762:LEU:HD12	2.00	0.43
2:B:60:GLN:OE1	2:B:60:GLN:HA	2.17	0.43
1:C:545:TRP:HA	1:C:546:PRO:HD3	1.68	0.43
1:C:647:LYS:HB2	1:C:675:TYR:CD2	2.53	0.43
1:G:439:GLU:HG3	1:G:440:ALA:N	2.33	0.43
1:G:484:ALA:O	1:G:487:SER:HB2	2.18	0.43
1:A:537:ILE:HD12	1:A:581:TRP:CH2	2.54	0.43
1:A:553:PHE:CE2	1:A:556:PRO:HD3	2.54	0.43
1:C:668:LEU:HD12	1:C:669:ILE:H	1.83	0.43
1:E:553:PHE:HZ	1:E:609:ALA:HB2	1.82	0.43
1:E:558:GLU:OE2	1:E:612:LEU:HD12	2.17	0.43
1:G:731:LEU:O	1:G:735:LEU:HG	2.19	0.43
1:E:577:ARG:HD2	2:F:33:TRP:CE3	2.53	0.43
2:H:45:CYS:O	2:H:46:ARG:HB2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:708:LYS:HE2	1:A:708:LYS:HB3	1.85	0.43
1:C:642:ILE:HD11	1:C:688:MET:CA	2.47	0.43
1:E:640:LEU:O	1:E:644:LEU:CD1	2.61	0.43
1:G:439:GLU:CG	1:G:440:ALA:H	2.30	0.43
1:A:689:LYS:HD3	1:A:689:LYS:HA	1.86	0.43
1:C:419:PRO:HG3	1:C:456:ILE:HG23	1.99	0.43
1:C:537:ILE:HG12	1:C:538:GLN:N	2.34	0.43
1:G:622:VAL:HB	1:G:664:LYS:O	2.19	0.43
1:A:456:ILE:O	1:A:459:LYS:HE3	2.18	0.43
1:E:725:LEU:HD12	1:E:725:LEU:HA	1.78	0.43
1:A:591:VAL:HG13	2:B:23:GLU:HB2	2.01	0.43
2:F:46:ARG:HG3	1:G:759:LYS:HE3	2.01	0.42
1:A:662:GLU:O	1:A:662:GLU:HG2	2.18	0.42
1:A:724:VAL:CG1	1:A:725:LEU:N	2.82	0.42
1:A:496:CYS:HB3	1:A:500:TYR:CB	2.49	0.42
1:E:493:LYS:HZ2	1:E:505:GLN:NE2	2.15	0.42
2:B:72:TRP:HB2	2:B:105:LYS:HG3	2.00	0.42
1:C:561:ARG:NH1	1:C:565:ARG:HE	2.17	0.42
1:E:426:CYS:O	1:E:430:LEU:HD13	2.19	0.42
1:E:602:GLN:CB	1:E:683:ASN:HD22	2.32	0.42
1:E:724:VAL:CG1	1:E:725:LEU:N	2.82	0.42
1:G:495:ALA:O	1:G:496:CYS:SG	2.73	0.42
2:B:49:ILE:H	2:B:49:ILE:HG12	1.65	0.42
1:C:419:PRO:O	1:C:462:PHE:HD1	2.02	0.42
1:C:479:SER:OG	1:C:485:GLU:OE2	2.34	0.42
1:G:453:PHE:CZ	1:G:459:LYS:HD2	2.55	0.42
1:G:470:LEU:O	1:G:470:LEU:CD2	2.68	0.42
1:A:643:LEU:HB3	1:A:649:LEU:HD12	2.02	0.42
1:A:751:LYS:O	1:A:755:ILE:HG13	2.20	0.42
1:C:610:ILE:CD1	1:C:643:LEU:HG	2.50	0.42
1:E:555:LEU:HD22	1:E:556:PRO:HD2	2.02	0.42
1:E:693:LYS:O	1:E:697:GLU:HG3	2.20	0.42
1:C:420:GLU:HG2	1:C:424:ARG:CD	2.49	0.42
1:E:463:GLN:OE1	1:E:500:TYR:HD1	2.03	0.42
1:E:604:SER:OG	1:E:607:GLN:HG3	2.19	0.42
1:E:610:ILE:HD12	1:E:611:LEU:HG	2.01	0.42
1:G:618:ASP:N	1:G:618:ASP:OD1	2.51	0.42
1:G:702:ASN:O	1:G:706:ASP:HB2	2.19	0.42
1:C:504:LEU:O	1:C:508:PHE:CE1	2.73	0.41
1:C:622:VAL:HB	1:C:665:PRO:HA	2.02	0.41
1:C:727:HIS:HB2	1:C:770:ASP:HB3	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:746:VAL:HB	1:C:747:PRO:HD3	2.01	0.41
1:E:492:LEU:HA	1:E:495:ALA:CB	2.36	0.41
1:E:430:LEU:HD23	1:E:485:GLU:OE1	2.19	0.41
2:F:41:ASN:ND2	2:H:97:ASP:HB3	2.35	0.41
1:G:610:ILE:O	1:G:613:GLN:HB2	2.20	0.41
1:C:489:ILE:HD11	1:C:508:PHE:CE1	2.54	0.41
1:E:535:PHE:CG	1:E:536:SER:N	2.88	0.41
1:E:589:GLU:HB2	2:F:26:LYS:HB2	2.01	0.41
1:E:597:ASN:HB2	1:E:599:TYR:HE1	1.83	0.41
1:G:710:LEU:O	1:G:713:ALA:HB3	2.20	0.41
1:A:560:GLU:HB3	1:C:564:GLN:OE1	2.21	0.41
1:E:460:ASP:OD1	1:E:460:ASP:N	2.54	0.41
1:A:466:TYR:HE2	1:A:473:ARG:HH22	1.67	0.41
2:B:49:ILE:HD13	2:D:37:ILE:CD1	2.50	0.41
1:C:533:LEU:HD22	2:D:24:VAL:CG1	2.49	0.41
1:C:540:LEU:HD13	1:C:545:TRP:CE2	2.54	0.41
1:E:743:LYS:HA	1:E:743:LYS:CE	2.46	0.41
2:F:74:VAL:HG13	2:F:102:GLU:HB2	2.03	0.41
1:G:746:VAL:N	1:G:747:PRO:CD	2.83	0.41
2:H:43:ALA:HB3	2:H:79:PHE:CE2	2.55	0.41
1:E:551:CYS:O	1:E:552:THR:C	2.59	0.41
1:E:590:LEU:CD2	2:F:24:VAL:HG22	2.51	0.41
1:E:761:TYR:HA	2:H:86:ARG:NH2	2.35	0.41
1:G:626:THR:OG1	1:G:636:LEU:HD23	2.20	0.41
1:G:633:MET:O	1:G:634:ASP:C	2.58	0.41
1:C:709:LEU:CD2	1:C:712:GLN:OE1	2.64	0.41
1:G:589:GLU:HB2	2:H:26:LYS:HB2	2.03	0.41
1:G:762:LEU:HD12	1:G:762:LEU:C	2.40	0.41
1:A:554:ALA:O	1:A:555:LEU:C	2.58	0.41
1:E:603:ALA:HB1	1:E:607:GLN:HB2	2.01	0.41
2:H:93:VAL:O	2:H:94:CYS:C	2.59	0.41
1:A:724:VAL:HG12	1:A:725:LEU:N	2.36	0.41
2:B:40:ASP:O	2:B:48:HIS:CD2	2.73	0.41
2:B:79:PHE:CE1	2:B:101:TRP:CZ3	3.09	0.41
1:E:529:GLU:HG2	1:E:565:ARG:NH1	2.35	0.41
1:G:511:ILE:O	1:G:515:LYS:HG3	2.21	0.41
1:C:554:ALA:HB2	1:C:630:GLN:HG3	2.02	0.40
1:G:464:LYS:HG3	1:G:699:THR:HG23	2.03	0.40
1:A:621:THR:OG1	1:A:624:GLN:HG3	2.21	0.40
1:A:755:ILE:HG23	2:B:93:VAL:HG11	2.02	0.40
1:C:470:LEU:HD11	1:C:508:PHE:CZ	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:553:PHE:HE1	1:C:631:ILE:HD11	1.86	0.40
1:C:694:GLN:O	1:C:698:THR:HG22	2.22	0.40
2:D:84:ILE:HD12	2:D:84:ILE:HA	1.93	0.40
1:E:451:GLU:O	1:E:455:LYS:HG3	2.20	0.40
1:E:608:MET:HE3	2:F:24:VAL:HG13	2.04	0.40
1:G:503:LYS:HE3	1:G:503:LYS:HB2	1.81	0.40
1:C:540:LEU:HB3	1:C:545:TRP:CD1	2.56	0.40
1:C:547:PHE:HB3	1:C:582:LEU:HD13	2.02	0.40
1:C:559:LEU:HD22	2:D:27:TRP:CE3	2.57	0.40
2:D:79:PHE:CZ	2:D:95:PRO:HD2	2.56	0.40
1:E:437:PRO:HB2	1:E:442:LEU:CD1	2.51	0.40
1:G:635:ILE:O	1:G:639:VAL:HG23	2.22	0.40
1:G:688:MET:H	1:G:688:MET:HG2	1.76	0.40
1:A:693:LYS:N	1:A:693:LYS:HD2	2.37	0.40
1:C:664:LYS:HA	1:C:665:PRO:HD3	1.90	0.40
1:E:750:LYS:O	1:E:753:ILE:HB	2.21	0.40
2:F:37:ILE:CD1	2:H:78:ALA:HB3	2.44	0.40
1:G:626:THR:HG1	1:G:633:MET:HG2	1.86	0.40
2:H:40:ASP:OD2	2:H:48:HIS:NE2	2.54	0.40
1:A:598:ARG:O	1:A:680:LEU:HD12	2.22	0.40
1:A:707:ARG:O	1:A:711:ILE:HG13	2.22	0.40
1:C:639:VAL:O	1:C:643:LEU:HD23	2.22	0.40
1:C:642:ILE:HD11	1:C:688:MET:CB	2.50	0.40
1:E:592:THR:HG22	2:F:22:PHE:CE2	2.57	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	349/368 (95%)	314 (90%)	31 (9%)	4 (1%)	14 50

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	C	299/368 (81%)	264 (88%)	30 (10%)	5 (2%)	9 40
1	E	357/368 (97%)	320 (90%)	30 (8%)	7 (2%)	7 36
1	G	358/368 (97%)	318 (89%)	35 (10%)	5 (1%)	11 45
2	B	84/106 (79%)	75 (89%)	8 (10%)	1 (1%)	13 48
2	D	75/106 (71%)	70 (93%)	5 (7%)	0	100 100
2	F	77/106 (73%)	72 (94%)	5 (6%)	0	100 100
2	H	77/106 (73%)	68 (88%)	6 (8%)	3 (4%)	3 20
All	All	1676/1896 (88%)	1501 (90%)	150 (9%)	25 (2%)	10 43

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	658	VAL
1	A	723	LYS
1	E	723	LYS
1	G	550	SER
1	A	480	ALA
1	C	721	MET
1	E	432	LYS
1	E	552	THR
1	E	653	ASP
1	G	723	LYS
1	A	727	HIS
2	B	62	SER
1	E	630	GLN
1	E	656	ALA
1	G	563	TYR
2	H	103	PHE
1	C	654	GLU
1	C	658	VAL
1	C	723	LYS
1	G	542	SER
1	G	608	MET
2	H	84	ILE
2	H	94	CYS
1	A	721	MET
1	C	546	PRO

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	323/339 (95%)	317 (98%)	6 (2%)	57 80
1	C	292/339 (86%)	283 (97%)	9 (3%)	40 71
1	E	328/339 (97%)	321 (98%)	7 (2%)	53 79
1	G	332/339 (98%)	323 (97%)	9 (3%)	44 74
2	B	76/90 (84%)	76 (100%)	0	100 100
2	D	70/90 (78%)	69 (99%)	1 (1%)	67 85
2	F	73/90 (81%)	72 (99%)	1 (1%)	67 85
2	H	71/90 (79%)	69 (97%)	2 (3%)	43 73
All	All	1565/1716 (91%)	1530 (98%)	35 (2%)	52 78

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	450	MET
1	A	574	HIS
1	A	600	THR
1	A	671	LEU
1	A	705	GLU
1	A	722	ARG
1	C	450	MET
1	C	470	LEU
1	C	542	SER
1	C	555	LEU
1	C	577	ARG
1	C	646	SER
1	C	705	GLU
1	C	743	LYS
1	C	762	LEU
2	D	68	CYS
1	E	517	LEU
1	E	555	LEU
1	E	645	LYS

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Mol	Chain	Res	Type
1	E	651	LEU
1	E	705	GLU
1	E	722	ARG
1	E	731	LEU
2	F	51	ASP
1	G	470	LEU
1	G	494	GLN
1	G	510	ASP
1	G	528	SER
1	G	536	SER
1	G	649	LEU
1	G	662	GLU
1	G	705	GLU
1	G	722	ARG
2	H	49	ILE
2	H	67	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	476	HIS
1	C	505	GLN
1	C	518	ASN
1	C	548	GLN
1	C	564	GLN
2	D	48	HIS
1	E	505	GLN
1	E	607	GLN
1	E	683	ASN
2	F	48	HIS
1	G	505	GLN
1	G	564	GLN
1	G	593	ASN
1	G	623	GLN
1	G	700	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 monosaccharides in this entry.

5.6 Ligand geometry

Of 12 ligands modelled in this entry, 12 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

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	353/368 (95%)	0.03	7 (1%)	65	52	63, 124, 177, 210	0
1	C	317/368 (86%)	0.27	16 (5%)	28	17	74, 155, 196, 213	0
1	E	359/368 (97%)	0.20	16 (4%)	33	21	80, 138, 180, 211	0
1	G	360/368 (97%)	0.10	9 (2%)	57	44	58, 124, 183, 217	0
2	B	86/106 (81%)	0.29	4 (4%)	31	20	64, 83, 183, 212	0
2	D	79/106 (74%)	0.04	1 (1%)	77	66	49, 78, 165, 220	0
2	F	81/106 (76%)	0.06	1 (1%)	79	68	61, 84, 142, 167	0
2	H	81/106 (76%)	0.19	4 (4%)	29	18	74, 102, 147, 168	0
All	All	1716/1896 (90%)	0.15	58 (3%)	45	31	49, 128, 186, 220	0

All (58) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	63	ALA	6.4
1	G	433	SER	5.8
2	B	65	SER	5.3
1	G	434	SER	5.2
2	B	62	SER	4.9
1	E	434	SER	4.1
2	F	106	TYR	3.8
1	C	668	LEU	3.8
1	E	658	VAL	3.8
2	B	64	THR	3.4
1	G	417	LYS	3.4
1	C	675	TYR	3.2
1	C	448	GLN	3.2
2	H	67	GLU	3.2
1	C	452	LYS	3.2
1	C	449	VAL	3.1

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Mol	Chain	Res	Type	RSRZ
1	E	659	ASP	3.1
2	D	106	TYR	3.0
1	E	616	THR	2.9
2	H	20	LYS	2.9
1	A	766	ASP	2.9
1	C	455	LYS	2.8
1	A	767	GLY	2.8
1	E	436	ASN	2.8
1	E	655	ASN	2.7
1	E	435	LYS	2.7
1	E	439	GLU	2.6
1	A	418	SER	2.6
1	G	436	ASN	2.6
1	A	448	GLN	2.5
2	H	104	GLN	2.5
1	E	657	ASN	2.5
1	C	689	LYS	2.4
1	C	667	THR	2.4
1	C	648	LEU	2.4
2	H	61	ALA	2.4
1	C	611	LEU	2.4
1	E	527	ASN	2.3
1	G	526	THR	2.3
1	G	528	SER	2.3
1	C	457	GLU	2.3
1	E	429	LEU	2.3
1	G	655	ASN	2.3
1	G	527	ASN	2.2
1	A	494	GLN	2.2
1	C	445	THR	2.2
1	E	437	PRO	2.2
1	C	558	GLU	2.2
1	C	767	GLY	2.2
1	C	519	GLU	2.2
1	E	500	TYR	2.2
1	A	528	SER	2.1
1	A	455	LYS	2.1
1	C	453	PHE	2.1
1	E	526	THR	2.1
1	E	769	LYS	2.1
1	E	444	ASP	2.1
1	G	657	ASN	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, 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	B-factors(Å^2)	Q<0.9
3	ZN	H	207	1/1	0.92	0.15	82,82,82,82	0
3	ZN	D	205	1/1	0.93	0.18	68,68,68,68	0
3	ZN	H	211	1/1	0.94	0.14	106,106,106,106	0
3	ZN	B	210	1/1	0.95	0.16	88,88,88,88	0
3	ZN	F	208	1/1	0.95	0.15	71,71,71,71	0
3	ZN	D	209	1/1	0.96	0.19	75,75,75,75	0
3	ZN	H	203	1/1	0.97	0.22	98,98,98,98	0
3	ZN	F	212	1/1	0.98	0.15	74,74,74,74	0
3	ZN	B	206	1/1	0.99	0.20	60,60,60,60	0
3	ZN	B	202	1/1	0.99	0.22	74,74,74,74	0
3	ZN	F	204	1/1	0.99	0.21	66,66,66,66	0
3	ZN	D	201	1/1	0.99	0.22	65,65,65,65	0

6.5 Other polymers (i)

There are no such residues in this entry.