



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 12:27 PM UTC

PDB ID : 2F9C / pdb_00002f9c
Title : Crystal structure of YDCK from Salmonella cholerae. NESG target SCR6
Authors : Benach, J.; Chen, Y.; Vorobiev, S.M.; Seetharaman, J.; Janjua, H.; Cooper, B.; Acton, X.T.B.; Montelione, G.T.; Hunt, J.F.; Tong, L.; Northeast Structural Genomics Consortium (NESG)
Deposited on : 2005-12-05
Resolution : 2.80 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
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

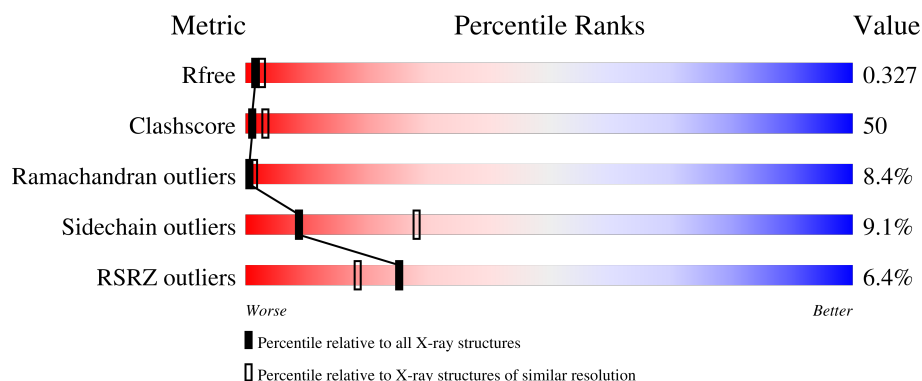
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	334	7% 30% 48% 15% • •
1	B	334	6% 29% 49% 15% • •

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5021 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 Hypothetical protein YDCK.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	320	Total	C	N	O	S	0	0	0
			2487	1546	452	481	8			
1	B	319	Total	C	N	O	S	0	0	0
			2478	1543	449	478	8			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	327	LEU	-	expression tag	GB 56413447
A	328	GLU	-	expression tag	GB 56413447
A	329	HIS	-	expression tag	GB 56413447
A	330	HIS	-	expression tag	GB 56413447
A	331	HIS	-	expression tag	GB 56413447
A	332	HIS	-	expression tag	GB 56413447
A	333	HIS	-	expression tag	GB 56413447
A	334	HIS	-	expression tag	GB 56413447
B	327	LEU	-	expression tag	GB 56413447
B	328	GLU	-	expression tag	GB 56413447
B	329	HIS	-	expression tag	GB 56413447
B	330	HIS	-	expression tag	GB 56413447
B	331	HIS	-	expression tag	GB 56413447
B	332	HIS	-	expression tag	GB 56413447
B	333	HIS	-	expression tag	GB 56413447
B	334	HIS	-	expression tag	GB 56413447

- Molecule 2 is CESIUM ION (CCD ID: CS) (formula: Cs).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	3	Total	Cs	0	0
			3	3		
2	B	3	Total	Cs	0	0
			3	3		

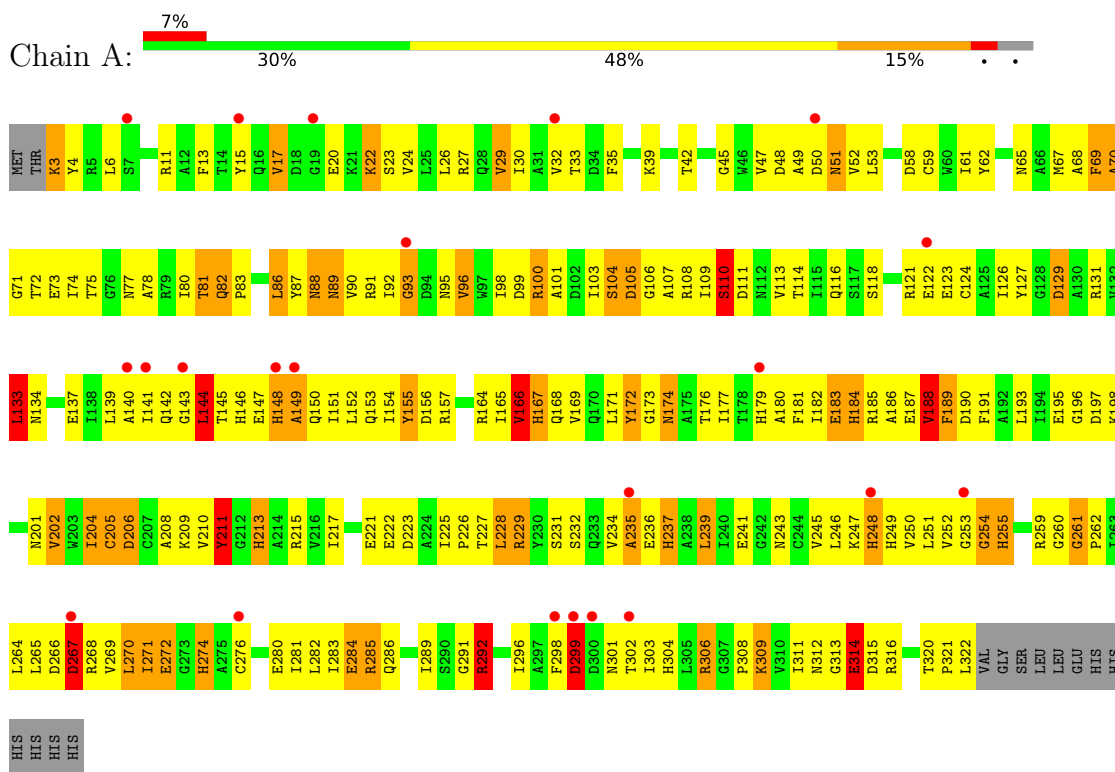
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	25	Total 25	O 25	0	0
3	B	25	Total 25	O 25	0	0

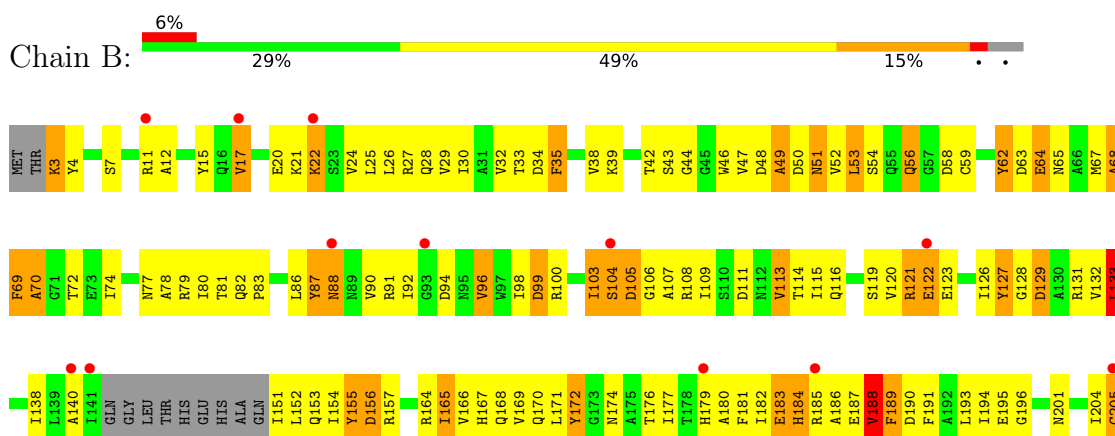
3 Residue-property plots [i](#)

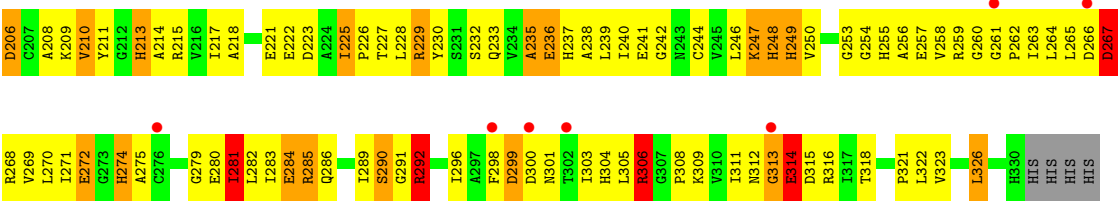
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Hypothetical protein YDCK



• Molecule 1: Hypothetical protein YDCK





4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	104.60Å 104.60Å 162.42Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.80 20.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	78.1 (20.00-2.80) 87.5 (20.00-2.80)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.87 (at 2.71Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.253 , 0.323 0.265 , 0.327	Depositor DCC
R_{free} test set	4488 reflections (9.80%)	wwPDB-VP
Wilson B-factor (Å ²)	41.8	Xtriage
Anisotropy	0.214	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 34.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	5021	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.67% of the height of the origin peak. No significant pseudotranslation is detected.*

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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section:
CS

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	0.50	0/2529	1.28	38/3435 (1.1%)
1	B	0.46	0/2519	1.24	38/3420 (1.1%)
All	All	0.48	0/5048	1.26	76/6855 (1.1%)

There are no bond length outliers.

All (76) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	213	HIS	N-CA-C	-12.62	95.14	112.30
1	B	213	HIS	N-CA-C	-11.69	97.80	112.88
1	A	274	HIS	N-CA-C	-11.46	97.51	112.41
1	A	229	ARG	N-CA-C	10.55	126.28	113.41
1	A	235	ALA	N-CA-C	10.55	128.78	114.12
1	B	229	ARG	N-CA-C	10.48	127.35	113.30
1	A	205	CYS	N-CA-C	10.34	125.54	108.48
1	A	284	GLU	N-CA-C	10.32	126.44	113.43
1	B	290	SER	N-CA-C	10.04	123.16	110.61
1	A	81	THR	N-CA-C	9.81	123.37	111.40
1	B	292	ARG	N-CA-C	-9.77	101.02	113.72
1	A	292	ARG	N-CA-C	-9.66	99.32	112.94
1	B	274	HIS	N-CA-C	-9.14	101.44	112.59
1	A	129	ASP	N-CA-C	-9.10	99.00	111.56
1	B	81	THR	N-CA-C	9.09	125.14	112.04
1	B	104	SER	N-CA-C	8.75	124.06	113.12
1	B	272	GLU	N-CA-C	8.67	125.67	114.75
1	B	174	ASN	N-CA-C	-8.35	100.59	113.02
1	B	129	ASP	N-CA-C	-8.26	101.35	112.26
1	B	69	PHE	N-CA-C	8.19	128.24	110.80
1	B	155	TYR	N-CA-C	8.11	125.31	108.53
1	A	155	TYR	N-CA-C	8.10	128.05	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	69	PHE	N-CA-C	7.91	125.86	114.39
1	A	189	PHE	N-CA-C	7.85	127.51	110.80
1	B	62	TYR	N-CA-C	7.62	122.33	112.89
1	B	233	GLN	N-CA-C	7.53	120.67	108.32
1	B	211	TYR	N-CA-C	7.47	125.02	112.99
1	B	172	TYR	N-CA-C	7.45	126.68	110.80
1	A	191	PHE	N-CA-C	-7.35	101.51	111.87
1	A	237	HIS	N-CA-C	-7.33	102.61	112.94
1	B	127	TYR	N-CA-C	7.31	125.75	114.64
1	B	121	ARG	N-CA-C	7.20	114.69	108.78
1	A	183	GLU	N-CA-C	7.14	126.01	110.80
1	B	284	GLU	N-CA-C	7.08	125.88	110.80
1	B	133	LEU	N-CA-C	7.02	118.43	108.74
1	A	95	ASN	N-CA-C	-6.91	104.16	112.59
1	A	174	ASN	N-CA-C	-6.90	101.18	111.81
1	B	189	PHE	N-CA-C	6.86	125.41	110.80
1	A	65	ASN	N-CA-C	-6.77	106.90	114.62
1	A	267	ASP	CB-CA-C	-6.56	108.99	116.54
1	B	183	GLU	N-CA-C	6.50	124.65	110.80
1	A	255	HIS	N-CA-C	-6.47	102.05	111.30
1	B	188	VAL	N-CA-C	-6.44	98.18	107.78
1	A	172	TYR	N-CA-C	6.38	124.40	110.80
1	B	191	PHE	N-CA-C	-6.34	104.17	112.41
1	B	225	ILE	N-CA-C	6.30	114.91	107.73
1	A	127	TYR	N-CA-C	6.19	123.68	114.09
1	B	154	ILE	N-CA-C	-6.15	96.91	107.24
1	A	166	VAL	N-CA-C	6.08	121.98	109.34
1	A	188	VAL	N-CA-C	-6.05	99.34	108.17
1	A	272	GLU	N-CA-C	5.97	122.60	112.99
1	A	211	TYR	N-CA-C	5.96	123.50	110.80
1	A	234	VAL	N-CA-C	-5.92	99.89	108.36
1	A	254	GLY	N-CA-C	-5.86	99.29	113.18
1	A	110	SER	N-CA-C	5.84	123.24	110.80
1	B	210	VAL	N-CA-C	-5.79	98.07	107.28
1	A	134	ASN	N-CA-C	5.76	118.22	111.02
1	A	298	PHE	N-CA-C	5.68	120.69	111.37
1	A	296	ILE	N-CA-C	5.66	116.15	107.77
1	A	196	GLY	N-CA-C	-5.61	104.47	112.55
1	B	87	TYR	N-CA-C	5.60	118.57	108.48
1	B	235	ALA	N-CA-C	5.60	122.73	110.80
1	B	121	ARG	CB-CA-C	-5.59	109.02	117.07
1	B	121	ARG	CA-C-O	5.57	121.17	117.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	281	ILE	N-CA-C	5.53	116.95	108.71
1	B	105	ASP	N-CA-C	5.53	116.92	108.30
1	B	51	ASN	N-CA-C	-5.52	99.05	110.80
1	B	195	GLU	N-CA-C	5.50	118.51	107.41
1	A	62	TYR	N-CA-C	5.47	118.30	111.24
1	A	133	LEU	N-CA-C	5.45	115.32	108.45
1	B	157	ARG	N-CA-C	-5.34	106.07	112.59
1	B	68	ALA	N-CA-C	-5.25	99.55	108.26
1	A	104	SER	N-CA-C	5.19	121.85	110.80
1	A	285	ARG	N-CA-C	5.14	121.76	110.80
1	A	204	ILE	N-CA-C	-5.08	100.43	107.80
1	B	103	ILE	N-CA-C	-5.03	102.25	108.89

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	2487	0	2425	242	0
1	B	2478	0	2422	266	0
2	A	3	0	0	0	0
2	B	3	0	0	0	0
3	A	25	0	0	4	0
3	B	25	0	0	7	0
All	All	5021	0	4847	488	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 50.

All (488) 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:A:105:ASP:HB2	1:A:122:GLU:HA	1.40	1.03
1:A:96:VAL:HG23	1:A:110:SER:O	1.60	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:70:ALA:HB3	1:A:88:ASN:N	1.81	0.96
1:A:106:GLY:O	1:A:123:GLU:HA	1.68	0.93
1:B:268:ARG:HE	1:B:286:GLN:HE21	1.06	0.92
1:B:228:LEU:HD21	1:B:246:LEU:HD12	1.55	0.88
1:A:156:ASP:HB2	1:A:172:TYR:O	1.74	0.88
1:B:286:GLN:O	1:B:308:PRO:HA	1.75	0.86
1:A:144:LEU:HD22	1:A:144:LEU:H	1.42	0.85
1:A:114:THR:HG21	1:A:131:ARG:HH21	1.45	0.82
1:A:103:ILE:HG12	1:A:109:ILE:HD11	1.60	0.82
1:B:114:THR:HG21	1:B:131:ARG:HH21	1.45	0.81
1:B:121:ARG:HG3	1:B:122:GLU:H	1.45	0.80
1:B:87:TYR:O	1:B:88:ASN:HB2	1.81	0.80
1:A:70:ALA:HB3	1:A:88:ASN:H	1.43	0.80
1:A:291:GLY:HA3	1:A:312:ASN:O	1.81	0.80
1:A:106:GLY:HA3	1:A:123:GLU:HG2	1.64	0.80
1:B:58:ASP:H	1:B:77:ASN:ND2	1.79	0.80
1:B:121:ARG:HG3	1:B:122:GLU:N	1.98	0.79
1:A:39:LYS:O	1:A:42:THR:HG22	1.81	0.79
1:B:52:VAL:HG13	1:B:72:THR:O	1.82	0.79
1:B:169:VAL:HG23	1:B:183:GLU:O	1.82	0.79
1:A:147:GLU:HB2	1:A:185:ARG:NH2	1.98	0.78
1:B:58:ASP:H	1:B:77:ASN:HD22	1.28	0.78
1:B:28:GLN:HE22	1:B:64:GLU:HG2	1.47	0.77
1:B:268:ARG:HE	1:B:286:GLN:NE2	1.81	0.76
1:A:91:ARG:HB2	1:A:108:ARG:HG2	1.66	0.76
1:A:193:LEU:HD23	1:A:215:ARG:HG2	1.67	0.76
1:A:48:ASP:HB2	1:A:69:PHE:HA	1.67	0.75
1:B:106:GLY:HA3	1:B:123:GLU:HG2	1.66	0.75
1:A:313:GLY:O	1:A:315:ASP:N	2.17	0.75
1:A:292:ARG:CB	1:A:292:ARG:HH11	2.01	0.74
1:B:122:GLU:HB2	1:B:140:ALA:O	1.88	0.74
1:A:99:ASP:O	1:A:100:ARG:HB2	1.87	0.74
1:B:237:HIS:HB2	1:B:254:GLY:O	1.87	0.73
1:A:274:HIS:HB3	1:B:131:ARG:HD2	1.71	0.73
1:B:166:VAL:HG12	1:B:167:HIS:H	1.53	0.72
1:A:251:LEU:HD23	1:A:251:LEU:C	2.14	0.72
1:B:169:VAL:HG22	1:B:186:ALA:HB3	1.72	0.72
1:A:152:LEU:HD12	1:A:166:VAL:O	1.90	0.72
1:B:59:CYS:HA	1:B:78:ALA:O	1.90	0.72
1:A:177:ILE:HD11	1:A:188:VAL:HG21	1.73	0.71
1:B:4:TYR:HA	1:B:32:VAL:HG23	1.71	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:75:THR:O	1:A:93:GLY:HA2	1.91	0.71
1:B:72:THR:HG23	1:B:90:VAL:HB	1.71	0.71
1:B:171:LEU:HD23	1:B:188:VAL:HG13	1.72	0.71
1:A:182:ILE:HG12	1:A:204:ILE:HD12	1.72	0.71
1:A:215:ARG:HD2	1:B:193:LEU:HD13	1.73	0.70
1:A:285:ARG:CZ	1:A:308:PRO:HD3	2.21	0.70
1:B:96:VAL:HG21	1:B:109:ILE:HG22	1.72	0.70
1:A:58:ASP:H	1:A:77:ASN:ND2	1.90	0.69
1:A:3:LYS:HB3	1:A:33:THR:CG2	2.23	0.69
1:B:170:GLN:HB2	1:B:187:GLU:HG2	1.74	0.69
1:B:236:GLU:HB2	1:B:254:GLY:N	2.08	0.68
1:A:272:GLU:O	1:A:272:GLU:HG2	1.93	0.68
1:B:121:ARG:CG	1:B:122:GLU:H	2.00	0.68
1:A:262:PRO:HD2	1:A:280:GLU:HB2	1.74	0.68
1:B:236:GLU:HB2	1:B:254:GLY:H	1.59	0.68
1:B:82:GLN:HB3	1:B:83:PRO:CD	2.23	0.68
1:B:228:LEU:HD23	1:B:246:LEU:HB2	1.75	0.67
1:A:3:LYS:HB3	1:A:33:THR:HG22	1.77	0.67
1:A:82:GLN:HB3	1:A:83:PRO:CD	2.25	0.67
1:A:267:ASP:HB2	1:A:284:GLU:O	1.95	0.67
1:A:292:ARG:HH11	1:A:292:ARG:HB2	1.59	0.67
1:A:241:GLU:OE2	1:A:259:ARG:HB2	1.94	0.67
1:A:301:ASN:HA	3:A:421:HOH:O	1.95	0.67
1:A:147:GLU:HB2	1:A:185:ARG:HH21	1.59	0.66
1:B:313:GLY:C	1:B:315:ASP:H	2.02	0.66
1:A:166:VAL:HG23	1:A:183:GLU:HG2	1.77	0.66
1:A:48:ASP:HB2	1:A:69:PHE:CA	2.23	0.66
1:B:53:LEU:HD23	1:B:54:SER:N	2.11	0.66
1:A:271:ILE:HD12	1:A:271:ILE:N	2.11	0.65
1:A:22:LYS:HE2	1:A:23:SER:H	1.60	0.65
1:A:169:VAL:HG21	1:A:182:ILE:HG22	1.78	0.65
1:B:114:THR:HG21	1:B:131:ARG:NH2	2.11	0.65
1:A:59:CYS:HA	1:A:78:ALA:O	1.95	0.65
1:B:115:ILE:HD13	1:B:132:VAL:HB	1.79	0.65
1:A:116:GLN:HE22	1:B:296:ILE:HD11	1.62	0.65
1:A:316:ARG:HD2	1:B:99:ASP:OD1	1.96	0.64
1:B:90:VAL:O	1:B:91:ARG:HD2	1.97	0.64
1:B:17:VAL:CG2	1:B:20:GLU:HB2	2.28	0.64
1:B:155:TYR:O	1:B:155:TYR:CD1	2.51	0.64
1:B:166:VAL:HG12	1:B:167:HIS:N	2.12	0.64
1:A:285:ARG:NH2	1:A:308:PRO:HD3	2.13	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:56:GLN:NE2	1:B:56:GLN:N	2.46	0.64
1:B:187:GLU:O	1:B:209:LYS:HA	1.97	0.64
1:A:169:VAL:HG23	1:A:183:GLU:O	1.97	0.64
1:A:171:LEU:HD23	1:A:188:VAL:HG13	1.80	0.64
1:B:111:ASP:HB2	1:B:127:TYR:O	1.98	0.64
1:A:11:ARG:HD2	1:A:13:PHE:CZ	2.33	0.64
1:A:100:ARG:HD2	1:A:100:ARG:O	1.97	0.63
1:A:152:LEU:C	1:A:152:LEU:HD23	2.23	0.63
1:A:313:GLY:C	1:A:315:ASP:H	2.04	0.63
1:A:260:GLY:O	1:A:261:GLY:O	2.16	0.63
1:A:148:HIS:O	1:A:150:GLN:N	2.30	0.63
1:A:131:ARG:HH11	1:B:274:HIS:HB3	1.64	0.62
1:A:166:VAL:CG2	1:A:183:GLU:HG2	2.28	0.62
1:B:281:ILE:HD12	1:B:281:ILE:N	2.14	0.62
1:B:260:GLY:HA3	1:B:279:GLY:H	1.64	0.62
1:B:270:LEU:CD2	1:B:272:GLU:HB2	2.28	0.62
1:A:155:TYR:HD1	1:A:155:TYR:O	1.83	0.62
1:A:52:VAL:HG22	1:A:72:THR:O	2.00	0.62
1:B:312:ASN:O	1:B:313:GLY:O	2.17	0.61
1:A:101:ALA:HB1	1:A:118:SER:O	2.00	0.61
1:B:306:ARG:H	1:B:326:LEU:CD2	2.14	0.61
1:B:189:PHE:O	1:B:189:PHE:HD1	1.84	0.61
1:B:70:ALA:HB3	1:B:88:ASN:H	1.65	0.61
1:B:103:ILE:HD12	1:B:103:ILE:N	2.14	0.61
1:A:86:LEU:HD23	1:A:86:LEU:N	2.15	0.61
1:A:205:CYS:HB3	3:A:417:HOH:O	2.01	0.60
1:B:176:THR:HB	1:B:193:LEU:HD12	1.82	0.60
1:B:206:ASP:CG	1:B:229:ARG:O	2.44	0.60
1:B:306:ARG:H	1:B:326:LEU:HD21	1.66	0.60
1:A:29:VAL:HB	1:A:45:GLY:O	2.01	0.60
1:A:155:TYR:O	1:A:155:TYR:CD1	2.55	0.60
1:B:103:ILE:CG2	1:B:107:ALA:HB3	2.32	0.60
1:A:99:ASP:OD1	1:B:316:ARG:HD2	2.02	0.60
1:A:86:LEU:HA	1:A:103:ILE:O	2.02	0.60
1:A:122:GLU:HG3	1:A:141:ILE:HD13	1.83	0.60
1:A:270:LEU:HD21	1:A:272:GLU:HB2	1.84	0.60
1:B:171:LEU:CD2	1:B:188:VAL:HG13	2.32	0.60
1:B:313:GLY:O	1:B:315:ASP:N	2.30	0.60
1:A:221:GLU:CD	1:A:221:GLU:H	2.10	0.60
1:A:58:ASP:H	1:A:77:ASN:HD22	1.50	0.59
1:A:50:ASP:O	1:A:51:ASN:HB2	2.00	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:87:TYR:O	1:A:88:ASN:HB2	2.02	0.59
1:A:73:GLU:HG3	1:A:91:ARG:NH1	2.18	0.59
1:B:306:ARG:HB2	1:B:326:LEU:HD22	1.85	0.59
1:A:285:ARG:HG3	1:A:306:ARG:CZ	2.33	0.59
1:B:177:ILE:N	1:B:177:ILE:HD12	2.18	0.59
1:A:70:ALA:HB3	1:A:88:ASN:CA	2.33	0.59
1:B:227:THR:HG22	1:B:229:ARG:HG3	1.85	0.59
1:A:206:ASP:OD2	1:A:229:ARG:O	2.20	0.58
1:B:56:GLN:NE2	1:B:56:GLN:H	2.02	0.58
1:B:167:HIS:HB3	1:B:168:GLN:OE1	2.03	0.58
1:B:44:GLY:O	1:B:64:GLU:HA	2.03	0.58
1:A:157:ARG:HG3	1:A:157:ARG:HH11	1.67	0.58
1:B:7:SER:HB2	1:B:28:GLN:HB3	1.85	0.58
1:B:152:LEU:HD23	1:B:152:LEU:C	2.29	0.58
1:B:261:GLY:O	1:B:263:ILE:HG13	2.03	0.58
1:A:148:HIS:O	1:A:149:ALA:C	2.47	0.57
1:B:109:ILE:HD13	1:B:115:ILE:HG13	1.85	0.57
1:B:152:LEU:HD23	1:B:153:GLN:N	2.19	0.57
1:A:253:GLY:O	1:A:272:GLU:HG3	2.03	0.57
1:B:70:ALA:HB3	1:B:88:ASN:N	2.19	0.57
1:B:4:TYR:CD1	1:B:29:VAL:HG13	2.39	0.57
1:B:304:HIS:HD2	1:B:305:LEU:N	2.03	0.57
1:B:230:TYR:C	1:B:232:SER:H	2.12	0.57
1:A:270:LEU:C	1:A:271:ILE:HD12	2.30	0.57
1:B:103:ILE:HG23	1:B:107:ALA:HB3	1.86	0.57
1:B:86:LEU:CD2	1:B:103:ILE:HD13	2.35	0.56
1:A:153:GLN:HB3	1:A:155:TYR:HD2	1.69	0.56
1:A:264:LEU:HB3	1:A:282:LEU:HD12	1.88	0.56
1:B:47:VAL:HG12	1:B:49:ALA:H	1.70	0.56
1:A:217:ILE:O	1:A:226:PRO:HG2	2.06	0.56
1:A:187:GLU:O	1:A:209:LYS:HA	2.06	0.56
1:B:68:ALA:HA	1:B:86:LEU:O	2.06	0.56
1:B:217:ILE:O	1:B:226:PRO:HG2	2.05	0.56
1:A:90:VAL:O	1:A:91:ARG:HD2	2.04	0.56
1:B:63:ASP:OD1	1:B:65:ASN:HB2	2.06	0.56
1:B:82:GLN:HB3	1:B:83:PRO:HD2	1.87	0.55
1:B:164:ARG:C	1:B:165:ILE:HD13	2.30	0.55
1:B:187:GLU:HB2	1:B:209:LYS:HG2	1.88	0.55
1:A:70:ALA:HB3	1:A:88:ASN:HA	1.88	0.55
1:A:285:ARG:HH21	1:A:286:GLN:NE2	2.04	0.55
1:B:86:LEU:HD22	1:B:103:ILE:HB	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:247:LYS:HB2	1:A:266:ASP:HA	1.88	0.55
1:B:47:VAL:CG1	1:B:48:ASP:N	2.69	0.55
1:A:103:ILE:N	1:A:103:ILE:HD12	2.22	0.55
1:A:195:GLU:CD	1:B:259:ARG:HH22	2.14	0.55
1:B:129:ASP:N	1:B:156:ASP:O	2.35	0.55
1:A:281:ILE:HG22	1:A:283:ILE:HG13	1.86	0.55
1:B:166:VAL:O	1:B:183:GLU:O	2.25	0.55
1:A:243:ASN:C	1:A:243:ASN:HD22	2.14	0.55
1:B:256:ALA:CB	1:B:271:ILE:HG22	2.37	0.55
1:A:13:PHE:O	1:A:23:SER:HA	2.07	0.55
1:B:168:GLN:HE21	1:B:185:ARG:NH1	2.05	0.55
1:B:222:GLU:HG2	1:B:223:ASP:OD1	2.07	0.55
1:B:268:ARG:NE	1:B:286:GLN:HE21	1.90	0.54
1:A:169:VAL:CG2	1:A:182:ILE:HG22	2.38	0.54
1:A:270:LEU:CD2	1:A:272:GLU:HB2	2.38	0.54
1:B:96:VAL:CG2	1:B:109:ILE:HG22	2.35	0.54
1:A:70:ALA:CB	1:A:88:ASN:HA	2.37	0.54
1:B:214:ALA:HB2	1:B:235:ALA:O	2.08	0.54
1:B:268:ARG:HG3	1:B:268:ARG:HH11	1.71	0.54
1:B:168:GLN:HE21	1:B:185:ARG:HH12	1.56	0.54
1:A:68:ALA:HA	1:A:86:LEU:O	2.08	0.54
1:B:189:PHE:O	1:B:189:PHE:CD1	2.60	0.54
1:A:116:GLN:NE2	1:B:296:ILE:HD11	2.23	0.54
1:A:227:THR:HB	1:A:245:VAL:HG22	1.88	0.54
1:A:49:ALA:O	1:A:50:ASP:C	2.50	0.54
1:B:86:LEU:HD21	1:B:103:ILE:HD13	1.89	0.54
1:A:91:ARG:CB	1:A:108:ARG:HG2	2.37	0.54
1:B:239:LEU:HB3	1:B:257:GLU:HG3	1.90	0.54
1:A:177:ILE:HD11	1:A:188:VAL:CG2	2.38	0.53
1:B:123:GLU:C	1:B:151:ILE:HD11	2.33	0.53
1:A:272:GLU:O	1:A:272:GLU:CG	2.56	0.53
1:A:280:GLU:C	1:A:281:ILE:HD12	2.33	0.53
1:B:228:LEU:CD2	1:B:246:LEU:HD12	2.33	0.53
1:B:299:ASP:C	1:B:301:ASN:N	2.63	0.53
1:A:157:ARG:HG3	1:A:157:ARG:NH1	2.23	0.53
1:A:193:LEU:CD2	1:A:215:ARG:HG2	2.37	0.53
1:A:285:ARG:HB2	1:A:306:ARG:O	2.09	0.53
1:A:281:ILE:HD12	1:A:281:ILE:N	2.23	0.53
1:B:28:GLN:CD	1:B:43:SER:HB2	2.32	0.53
1:A:3:LYS:HB2	1:A:3:LYS:NZ	2.23	0.53
1:A:144:LEU:H	1:A:144:LEU:CD2	2.17	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:180:ALA:C	1:A:181:PHE:HD2	2.16	0.53
1:B:290:SER:O	1:B:290:SER:OG	2.22	0.53
1:A:87:TYR:O	1:A:88:ASN:CB	2.56	0.53
1:A:105:ASP:N	1:A:121:ARG:O	2.41	0.53
1:A:137:GLU:CD	1:A:164:ARG:HH21	2.17	0.53
1:A:172:TYR:CE1	1:A:189:PHE:HB2	2.43	0.53
1:B:87:TYR:O	1:B:104:SER:O	2.26	0.53
1:B:11:ARG:HG2	1:B:12:ALA:H	1.73	0.52
1:B:229:ARG:NH1	1:B:247:LYS:HE2	2.24	0.52
1:B:268:ARG:HG3	1:B:268:ARG:NH1	2.24	0.52
1:B:91:ARG:HB2	1:B:108:ARG:HG2	1.90	0.52
1:B:108:ARG:HG3	1:B:108:ARG:HH11	1.74	0.52
1:B:267:ASP:HB2	1:B:284:GLU:O	2.09	0.52
1:A:151:ILE:O	1:A:153:GLN:HG3	2.08	0.52
1:A:264:LEU:C	1:A:265:LEU:HD23	2.34	0.52
1:A:88:ASN:HB2	1:A:104:SER:O	2.09	0.52
1:B:306:ARG:CB	1:B:326:LEU:HD22	2.39	0.52
1:A:241:GLU:O	1:A:259:ARG:HA	2.09	0.52
1:A:129:ASP:HB3	1:B:274:HIS:HE1	1.75	0.52
1:B:120:VAL:HA	1:B:138:ILE:HB	1.92	0.52
1:A:82:GLN:CB	1:A:83:PRO:CD	2.88	0.52
1:B:27:ARG:NE	3:B:408:HOH:O	2.42	0.52
1:B:269:VAL:HG12	1:B:271:ILE:HD12	1.92	0.52
1:B:32:VAL:HG12	1:B:32:VAL:O	2.09	0.52
1:B:314:GLU:H	1:B:314:GLU:CD	2.18	0.52
1:B:44:GLY:HA3	3:B:425:HOH:O	2.09	0.51
1:B:312:ASN:ND2	1:B:313:GLY:H	2.08	0.51
1:A:47:VAL:CG1	1:A:52:VAL:HB	2.39	0.51
1:B:70:ALA:HB3	1:B:88:ASN:CA	2.41	0.51
1:B:215:ARG:HB2	1:B:239:LEU:HD23	1.92	0.51
1:B:256:ALA:HB1	1:B:271:ILE:HG22	1.91	0.51
1:B:291:GLY:HA3	1:B:312:ASN:O	2.10	0.51
1:A:248:HIS:HB3	1:A:249:HIS:HD2	1.75	0.51
1:B:28:GLN:NE2	1:B:43:SER:HB2	2.24	0.51
1:B:35:PHE:CD1	1:B:35:PHE:N	2.79	0.51
1:A:98:ILE:HD13	1:A:103:ILE:HD13	1.93	0.51
1:B:266:ASP:O	1:B:267:ASP:C	2.53	0.51
1:A:89:ASN:O	1:A:91:ARG:HD3	2.11	0.50
1:A:215:ARG:HD2	1:B:193:LEU:CD1	2.41	0.50
1:B:88:ASN:ND2	1:B:105:ASP:OD1	2.44	0.50
1:B:303:ILE:HD11	1:B:318:THR:HA	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:303:ILE:HA	1:A:320:THR:OG1	2.12	0.50
1:B:156:ASP:OD2	1:B:172:TYR:O	2.29	0.50
1:B:272:GLU:HB3	1:B:290:SER:HB2	1.93	0.50
1:A:284:GLU:OE1	1:A:306:ARG:HD2	2.11	0.50
1:A:48:ASP:CB	1:A:69:PHE:HA	2.39	0.50
1:A:140:ALA:HB2	1:A:152:LEU:HD13	1.94	0.50
1:A:167:HIS:HB2	1:A:184:HIS:HA	1.94	0.50
1:A:131:ARG:HD2	1:B:274:HIS:HB3	1.93	0.50
1:A:264:LEU:O	1:A:265:LEU:HD23	2.11	0.50
1:B:133:LEU:HD23	1:B:133:LEU:N	2.26	0.50
1:B:313:GLY:C	1:B:315:ASP:N	2.70	0.50
1:B:299:ASP:C	1:B:301:ASN:H	2.19	0.50
1:A:74:ILE:HD13	1:A:80:ILE:CD1	2.42	0.50
1:A:113:VAL:CG1	1:A:114:THR:N	2.75	0.50
1:B:22:LYS:HE2	1:B:22:LYS:HA	1.93	0.50
1:B:305:LEU:HD13	1:B:311:ILE:CD1	2.42	0.50
1:A:270:LEU:HD23	1:A:271:ILE:N	2.27	0.50
1:A:82:GLN:HB3	1:A:83:PRO:HD2	1.94	0.49
1:B:100:ARG:O	1:B:100:ARG:HG2	2.12	0.49
1:A:313:GLY:C	1:A:315:ASP:N	2.65	0.49
1:A:237:HIS:HB2	1:A:254:GLY:O	2.12	0.49
1:B:184:HIS:CD2	1:B:184:HIS:N	2.80	0.49
1:A:4:TYR:HB2	1:A:30:ILE:O	2.13	0.49
1:A:167:HIS:HB3	1:A:168:GLN:OE1	2.12	0.49
1:A:271:ILE:HA	1:A:289:ILE:O	2.12	0.49
1:B:103:ILE:N	1:B:103:ILE:CD1	2.74	0.49
1:B:281:ILE:HG22	1:B:283:ILE:HG13	1.94	0.49
1:B:63:ASP:C	1:B:65:ASN:H	2.21	0.49
1:B:267:ASP:HB2	1:B:285:ARG:HA	1.95	0.49
1:A:145:THR:HG22	1:A:145:THR:O	2.13	0.49
1:B:285:ARG:NH1	3:B:419:HOH:O	2.45	0.49
1:B:86:LEU:HD23	1:B:103:ILE:H	1.78	0.49
1:A:103:ILE:CG2	1:A:107:ALA:HB3	2.42	0.48
1:A:156:ASP:CB	1:A:172:TYR:O	2.56	0.48
1:A:285:ARG:HG3	1:A:306:ARG:NH2	2.28	0.48
1:B:90:VAL:HG13	1:B:103:ILE:HG21	1.94	0.48
1:B:53:LEU:HD23	1:B:54:SER:H	1.78	0.48
1:B:312:ASN:CG	1:B:313:GLY:H	2.22	0.48
1:B:194:ILE:CD1	1:B:204:ILE:HD11	2.43	0.48
1:A:124:CYS:HA	1:A:151:ILE:CG1	2.44	0.48
1:A:92:ILE:HG23	1:A:96:VAL:HG11	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:144:LEU:HD22	1:A:144:LEU:N	2.21	0.48
1:A:172:TYR:CD1	1:A:189:PHE:HB2	2.49	0.48
1:A:282:LEU:HD23	1:A:304:HIS:CD2	2.48	0.48
1:B:188:VAL:HA	1:B:210:VAL:O	2.14	0.48
1:A:285:ARG:NH2	1:A:286:GLN:NE2	2.62	0.48
1:B:4:TYR:HB2	1:B:30:ILE:O	2.14	0.48
1:B:87:TYR:O	1:B:88:ASN:CB	2.59	0.48
1:B:3:LYS:HB2	1:B:3:LYS:NZ	2.29	0.48
1:B:168:GLN:NE2	1:B:185:ARG:NH1	2.62	0.48
1:B:182:ILE:HA	1:B:204:ILE:O	2.14	0.47
1:A:122:GLU:HB2	1:A:140:ALA:O	2.14	0.47
1:A:292:ARG:HB2	1:A:292:ARG:NH1	2.28	0.47
1:B:91:ARG:CB	1:B:108:ARG:HG2	2.44	0.47
1:A:227:THR:HG22	1:A:229:ARG:HG3	1.96	0.47
1:A:92:ILE:HG12	1:A:109:ILE:HD12	1.97	0.47
1:A:47:VAL:HG12	1:A:48:ASP:N	2.28	0.47
1:A:81:THR:HB	1:A:82:GLN:HE21	1.78	0.47
1:A:235:ALA:O	1:A:236:GLU:HG3	2.14	0.47
1:B:182:ILE:HG22	1:B:186:ALA:HB3	1.96	0.47
1:B:184:HIS:HB2	1:B:206:ASP:O	2.14	0.47
1:B:237:HIS:CB	1:B:254:GLY:O	2.62	0.47
1:B:249:HIS:CD2	3:B:409:HOH:O	2.67	0.47
1:B:92:ILE:HD13	1:B:98:ILE:HD12	1.95	0.47
1:A:106:GLY:C	1:A:123:GLU:HA	2.38	0.47
1:A:153:GLN:HB3	1:A:155:TYR:CD2	2.48	0.47
1:A:186:ALA:HB1	1:A:204:ILE:HG22	1.96	0.47
1:A:321:PRO:O	1:A:322:LEU:HG	2.15	0.47
1:B:38:VAL:HG13	1:B:42:THR:HG21	1.97	0.47
1:B:155:TYR:O	1:B:156:ASP:CG	2.58	0.47
1:A:267:ASP:HB3	1:A:268:ARG:H	1.45	0.47
1:B:47:VAL:HG12	1:B:49:ALA:N	2.29	0.47
1:B:240:ILE:HD13	1:B:258:VAL:HB	1.97	0.47
1:B:266:ASP:O	1:B:269:VAL:HG23	2.14	0.47
1:A:70:ALA:CB	1:A:88:ASN:N	2.68	0.47
1:A:104:SER:HB2	1:A:121:ARG:HA	1.96	0.47
1:B:90:VAL:HG22	1:B:103:ILE:HG22	1.95	0.47
1:B:246:LEU:HD22	1:B:265:LEU:HD12	1.96	0.47
1:B:25:LEU:O	1:B:26:LEU:HD23	2.15	0.46
1:B:217:ILE:HG22	1:B:218:ALA:N	2.30	0.46
1:A:6:LEU:HD22	1:A:27:ARG:HB2	1.97	0.46
1:A:285:ARG:HH21	1:A:286:GLN:CD	2.24	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:74:ILE:HD13	1:B:80:ILE:CD1	2.46	0.46
1:A:171:LEU:CD2	1:A:188:VAL:HG13	2.45	0.46
1:B:69:PHE:CD2	1:B:69:PHE:N	2.84	0.46
1:B:312:ASN:ND2	1:B:313:GLY:N	2.64	0.46
1:B:69:PHE:CZ	1:B:87:TYR:HB3	2.50	0.46
1:A:195:GLU:OE1	1:B:259:ARG:NH2	2.46	0.46
1:B:63:ASP:OD1	1:B:65:ASN:N	2.49	0.46
1:A:198:LYS:NZ	1:B:221:GLU:HG3	2.31	0.46
1:B:113:VAL:CG1	1:B:114:THR:N	2.78	0.46
1:B:241:GLU:CD	1:B:241:GLU:C	2.84	0.46
1:B:169:VAL:HG21	1:B:182:ILE:HG22	1.98	0.46
1:A:131:ARG:HB3	1:A:133:LEU:HD21	1.97	0.45
1:A:281:ILE:CG2	1:A:283:ILE:HG13	2.45	0.45
1:A:289:ILE:HA	1:A:311:ILE:O	2.15	0.45
1:A:316:ARG:HG2	1:A:316:ARG:HH11	1.81	0.45
1:B:289:ILE:HA	1:B:311:ILE:O	2.15	0.45
1:A:213:HIS:HE1	1:B:213:HIS:CE1	2.34	0.45
1:B:58:ASP:N	1:B:77:ASN:ND2	2.57	0.45
1:B:304:HIS:C	1:B:304:HIS:CD2	2.94	0.45
1:A:179:HIS:O	1:A:202:VAL:HG23	2.16	0.45
1:A:72:THR:HG23	1:A:90:VAL:HB	1.98	0.45
1:A:98:ILE:HD13	1:A:103:ILE:CD1	2.47	0.45
1:A:152:LEU:C	1:A:152:LEU:CD2	2.90	0.45
1:A:314:GLU:HG3	1:B:79:ARG:HE	1.82	0.45
1:B:164:ARG:HG2	1:B:181:PHE:CD2	2.51	0.45
1:B:241:GLU:CD	1:B:242:GLY:N	2.75	0.45
1:B:15:TYR:HE2	1:B:24:VAL:HG13	1.81	0.45
1:A:157:ARG:NH1	3:A:420:HOH:O	2.47	0.45
1:A:246:LEU:N	1:A:246:LEU:HD23	2.31	0.45
1:A:87:TYR:O	1:A:104:SER:O	2.35	0.45
1:A:232:SER:HA	1:A:250:VAL:O	2.17	0.45
1:A:274:HIS:CB	1:B:131:ARG:HD2	2.44	0.45
1:B:281:ILE:N	1:B:281:ILE:CD1	2.80	0.45
1:A:15:TYR:CE2	1:A:22:LYS:HB3	2.52	0.45
1:B:304:HIS:CD2	1:B:305:LEU:N	2.84	0.45
1:A:174:ASN:OD1	1:B:255:HIS:CE1	2.70	0.44
1:B:28:GLN:NE2	1:B:64:GLU:HG2	2.25	0.44
1:B:38:VAL:HB	3:B:407:HOH:O	2.18	0.44
1:B:292:ARG:HH12	1:B:314:GLU:HB3	1.82	0.44
1:A:103:ILE:CG1	1:A:109:ILE:HD11	2.39	0.44
1:B:322:LEU:C	1:B:323:VAL:HG13	2.42	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:6:LEU:HD11	1:A:50:ASP:H	1.82	0.44
1:A:74:ILE:HD13	1:A:80:ILE:HD12	2.00	0.44
1:A:251:LEU:HD23	1:A:252:VAL:N	2.32	0.44
1:B:285:ARG:HG3	1:B:306:ARG:NH2	2.32	0.44
1:B:67:MET:HB3	1:B:69:PHE:CE2	2.53	0.44
1:B:151:ILE:N	3:B:410:HOH:O	2.50	0.44
1:A:4:TYR:CD1	1:A:4:TYR:C	2.95	0.44
1:A:188:VAL:HA	1:A:210:VAL:O	2.17	0.44
1:B:56:GLN:N	1:B:56:GLN:CD	2.76	0.44
1:B:113:VAL:HG11	1:B:126:ILE:CG2	2.48	0.44
1:A:71:GLY:O	1:A:91:ARG:NH1	2.44	0.44
1:A:316:ARG:HG2	1:A:316:ARG:NH1	2.33	0.44
1:B:77:ASN:O	1:B:78:ALA:C	2.60	0.44
1:B:249:HIS:CD2	1:B:249:HIS:H	2.35	0.44
1:B:306:ARG:HH11	1:B:306:ARG:HG2	1.83	0.44
1:B:256:ALA:HB1	1:B:271:ILE:CG2	2.48	0.43
1:A:174:ASN:N	1:A:190:ASP:O	2.45	0.43
1:B:249:HIS:CD2	1:B:249:HIS:N	2.86	0.43
1:A:4:TYR:HA	1:A:32:VAL:HG23	2.00	0.43
1:A:271:ILE:N	1:A:271:ILE:CD1	2.81	0.43
1:B:165:ILE:HG22	1:B:169:VAL:HB	2.00	0.43
1:B:166:VAL:CG1	1:B:167:HIS:H	2.27	0.43
1:A:149:ALA:O	1:A:151:ILE:N	2.51	0.43
1:A:247:LYS:HE3	1:A:264:LEU:HD11	2.00	0.43
1:A:17:VAL:CG2	1:A:20:GLU:HB2	2.49	0.43
1:A:48:ASP:OD2	1:A:69:PHE:O	2.37	0.43
1:B:47:VAL:HG12	1:B:48:ASP:N	2.33	0.43
1:A:309:LYS:HB2	1:A:309:LYS:NZ	2.33	0.43
1:B:171:LEU:CD2	1:B:188:VAL:CG1	2.96	0.43
1:A:126:ILE:HG23	1:A:154:ILE:HB	2.00	0.43
1:A:299:ASP:C	1:A:301:ASN:H	2.27	0.43
1:B:74:ILE:HD13	1:B:80:ILE:HD12	2.00	0.43
1:B:238:ALA:HB2	1:B:253:GLY:HA2	2.01	0.43
1:B:90:VAL:HG12	1:B:91:ARG:N	2.33	0.43
1:B:230:TYR:C	1:B:232:SER:N	2.76	0.43
1:B:240:ILE:HA	1:B:258:VAL:O	2.19	0.43
1:A:61:ILE:HA	1:A:80:ILE:HB	2.01	0.43
1:A:261:GLY:N	3:A:409:HOH:O	2.52	0.43
1:B:33:THR:HG23	1:B:34:ASP:N	2.33	0.43
1:B:48:ASP:HB2	1:B:69:PHE:CA	2.49	0.43
1:A:88:ASN:C	1:A:90:VAL:N	2.71	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:190:ASP:OD2	1:A:211:TYR:O	2.37	0.42
1:B:206:ASP:HB2	1:B:230:TYR:HA	2.01	0.42
1:B:248:HIS:O	1:B:250:VAL:N	2.52	0.42
1:A:316:ARG:HD2	1:B:99:ASP:CG	2.43	0.42
1:B:49:ALA:O	1:B:50:ASP:C	2.61	0.42
1:B:280:GLU:O	1:B:280:GLU:HG2	2.19	0.42
1:B:153:GLN:HB2	1:B:170:GLN:NE2	2.34	0.42
1:B:306:ARG:HH11	1:B:306:ARG:CG	2.32	0.42
1:B:312:ASN:CG	1:B:313:GLY:N	2.78	0.42
1:A:228:LEU:N	1:A:228:LEU:HD23	2.34	0.42
1:B:113:VAL:HG12	1:B:114:THR:N	2.34	0.42
1:B:274:HIS:O	1:B:275:ALA:C	2.63	0.42
1:B:48:ASP:CB	1:B:69:PHE:O	2.68	0.42
1:B:176:THR:C	1:B:177:ILE:HD12	2.44	0.42
1:A:103:ILE:HG23	1:A:107:ALA:HB3	2.01	0.42
1:A:121:ARG:HB3	1:A:139:LEU:HD12	2.02	0.42
1:A:140:ALA:HB2	1:A:152:LEU:CD1	2.50	0.42
1:A:225:ILE:O	1:A:226:PRO:C	2.63	0.42
1:B:179:HIS:O	1:B:196:GLY:HA3	2.20	0.42
1:B:321:PRO:O	1:B:326:LEU:HG	2.20	0.42
1:B:248:HIS:HB3	1:B:249:HIS:H	1.59	0.42
1:A:182:ILE:HA	1:A:204:ILE:O	2.20	0.42
1:A:215:ARG:CD	1:B:193:LEU:HD22	2.49	0.42
1:A:222:GLU:HG2	1:A:223:ASP:OD1	2.20	0.42
1:A:237:HIS:CD2	1:A:255:HIS:CE1	3.08	0.42
1:B:28:GLN:N	1:B:46:TRP:CE3	2.88	0.42
1:B:169:VAL:CG2	1:B:182:ILE:HG22	2.50	0.42
1:B:184:HIS:CD2	1:B:184:HIS:H	2.37	0.42
1:A:73:GLU:CD	1:A:91:ARG:NH2	2.78	0.41
1:A:90:VAL:HG13	1:A:103:ILE:HG21	2.02	0.41
1:B:109:ILE:CD1	1:B:115:ILE:HG13	2.49	0.41
1:B:264:LEU:HD23	1:B:282:LEU:CD1	2.50	0.41
1:A:152:LEU:HD23	1:A:153:GLN:N	2.36	0.41
1:A:270:LEU:C	1:A:270:LEU:CD2	2.93	0.41
1:B:165:ILE:HD13	1:B:165:ILE:N	2.34	0.41
1:B:306:ARG:NE	3:B:420:HOH:O	2.52	0.41
1:A:165:ILE:N	1:A:165:ILE:HD13	2.35	0.41
1:B:180:ALA:C	1:B:181:PHE:HD2	2.27	0.41
1:A:124:CYS:HA	1:A:151:ILE:HG12	2.02	0.41
1:B:39:LYS:HD2	1:B:39:LYS:HA	1.89	0.41
1:B:108:ARG:HG3	1:B:108:ARG:NH1	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:285:ARG:NH2	1:B:286:GLN:OE1	2.53	0.41
1:B:299:ASP:HB3	1:B:300:ASP:H	1.66	0.41
1:A:88:ASN:O	1:A:90:VAL:N	2.54	0.41
1:A:239:LEU:C	1:A:239:LEU:HD13	2.45	0.41
1:B:116:GLN:O	1:B:133:LEU:HA	2.19	0.41
1:B:166:VAL:HB	1:B:167:HIS:ND1	2.36	0.41
1:A:266:ASP:O	1:A:269:VAL:HG23	2.19	0.41
1:B:194:ILE:HD11	1:B:204:ILE:HD11	2.02	0.41
1:B:226:PRO:HA	1:B:244:CYS:O	2.21	0.41
1:A:215:ARG:CD	1:B:193:LEU:HD13	2.46	0.41
1:B:104:SER:HB2	1:B:121:ARG:HA	2.01	0.41
1:A:122:GLU:CG	1:A:141:ILE:HD13	2.51	0.41
1:A:180:ALA:CB	1:A:202:VAL:HB	2.51	0.41
1:A:190:ASP:HB2	1:A:211:TYR:O	2.21	0.41
1:A:284:GLU:OE1	1:A:304:HIS:NE2	2.54	0.41
1:B:4:TYR:OH	1:B:53:LEU:O	2.39	0.41
1:B:62:TYR:CE1	1:B:79:ARG:HG2	2.55	0.41
1:B:86:LEU:HD13	1:B:92:ILE:CD1	2.51	0.41
1:B:267:ASP:HB3	1:B:268:ARG:H	1.51	0.41
1:B:201:ASN:O	1:B:225:ILE:HG23	2.21	0.41
1:A:48:ASP:HB2	1:A:69:PHE:CB	2.51	0.40
1:A:215:ARG:HB2	1:A:239:LEU:HD22	2.04	0.40
1:A:26:LEU:CD1	1:A:67:MET:HG2	2.50	0.40
1:A:88:ASN:O	1:A:89:ASN:C	2.64	0.40
1:A:179:HIS:ND1	1:A:197:ASP:HA	2.37	0.40
1:B:205:CYS:HB2	1:B:206:ASP:H	1.63	0.40
1:B:48:ASP:O	1:B:49:ALA:HB2	2.22	0.40
1:B:208:ALA:HA	1:B:232:SER:O	2.21	0.40
1:B:267:ASP:CB	1:B:285:ARG:HA	2.52	0.40
1:B:269:VAL:HG12	1:B:270:LEU:N	2.35	0.40
1:A:47:VAL:HG11	1:A:52:VAL:HB	2.04	0.40
1:A:168:GLN:HE21	1:A:185:ARG:NH1	2.18	0.40
1:A:201:ASN:HB3	1:A:202:VAL:H	1.77	0.40
1:B:180:ALA:O	1:B:181:PHE:HD2	2.04	0.40
1:B:322:LEU:O	1:B:323:VAL:CG1	2.69	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	318/334 (95%)	231 (73%)	61 (19%)	26 (8%)	0	1
1	B	315/334 (94%)	220 (70%)	68 (22%)	27 (9%)	0	1
All	All	633/668 (95%)	451 (71%)	129 (20%)	53 (8%)	0	1

All (53) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	51	ASN
1	A	88	ASN
1	A	100	ARG
1	A	111	ASP
1	A	144	LEU
1	A	149	ALA
1	A	167	HIS
1	A	206	ASP
1	A	248	HIS
1	A	314	GLU
1	B	51	ASN
1	B	88	ASN
1	B	122	GLU
1	B	156	ASP
1	B	184	HIS
1	B	206	ASP
1	B	236	GLU
1	B	248	HIS
1	B	249	HIS
1	B	285	ARG
1	A	17	VAL
1	A	143	GLY
1	A	166	VAL
1	A	184	HIS
1	A	208	ALA

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Mol	Chain	Res	Type
1	A	261	GLY
1	B	64	GLU
1	B	113	VAL
1	B	247	LYS
1	B	267	ASP
1	B	298	PHE
1	B	306	ARG
1	B	313	GLY
1	B	314	GLU
1	A	105	ASP
1	A	148	HIS
1	B	49	ALA
1	B	70	ALA
1	A	146	HIS
1	A	211	TYR
1	A	82	GLN
1	A	89	ASN
1	A	299	ASP
1	B	17	VAL
1	B	99	ASP
1	B	190	ASP
1	A	70	ALA
1	B	94	ASP
1	A	93	GLY
1	B	96	VAL
1	A	173	GLY
1	B	128	GLY
1	B	262	PRO

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	264/277 (95%)	235 (89%)	29 (11%)	6	20
1	B	264/277 (95%)	245 (93%)	19 (7%)	13	39
All	All	528/554 (95%)	480 (91%)	48 (9%)	9	28

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	LYS
1	A	22	LYS
1	A	24	VAL
1	A	29	VAL
1	A	35	PHE
1	A	53	LEU
1	A	86	LEU
1	A	96	VAL
1	A	110	SER
1	A	133	LEU
1	A	142	GLN
1	A	144	LEU
1	A	166	VAL
1	A	176	THR
1	A	188	VAL
1	A	202	VAL
1	A	228	LEU
1	A	231	SER
1	A	239	LEU
1	A	267	ASP
1	A	270	LEU
1	A	271	ILE
1	A	276	CYS
1	A	292	ARG
1	A	299	ASP
1	A	302	THR
1	A	306	ARG
1	A	309	LYS
1	A	314	GLU
1	B	3	LYS
1	B	21	LYS
1	B	22	LYS
1	B	35	PHE
1	B	53	LEU
1	B	56	GLN
1	B	119	SER
1	B	133	LEU
1	B	165	ILE
1	B	188	VAL
1	B	205	CYS
1	B	267	ASP
1	B	281	ILE

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Mol	Chain	Res	Type
1	B	292	ARG
1	B	299	ASP
1	B	306	ARG
1	B	309	LYS
1	B	314	GLU
1	B	326	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	16	GLN
1	A	36	ASN
1	A	56	GLN
1	A	77	ASN
1	A	82	GLN
1	A	95	ASN
1	A	116	GLN
1	A	134	ASN
1	A	142	GLN
1	A	168	GLN
1	A	213	HIS
1	A	237	HIS
1	A	243	ASN
1	A	249	HIS
1	A	255	HIS
1	A	286	GLN
1	A	301	ASN
1	B	16	GLN
1	B	28	GLN
1	B	56	GLN
1	B	77	ASN
1	B	88	ASN
1	B	116	GLN
1	B	134	ASN
1	B	135	GLN
1	B	170	GLN
1	B	200	ASN
1	B	201	ASN
1	B	213	HIS
1	B	237	HIS
1	B	243	ASN
1	B	248	HIS

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Mol	Chain	Res	Type
1	B	249	HIS
1	B	255	HIS
1	B	274	HIS
1	B	286	GLN
1	B	301	ASN
1	B	304	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 6 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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	320/334 (95%)	0.61	22 (6%) 23 16	17, 34, 58, 67	0
1	B	319/334 (95%)	0.51	19 (5%) 27 21	18, 34, 58, 68	0
All	All	639/668 (95%)	0.56	41 (6%) 25 18	17, 34, 58, 68	0

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	148	HIS	6.8
1	A	149	ALA	6.5
1	A	122	GLU	5.6
1	B	300	ASP	4.3
1	A	300	ASP	4.1
1	A	298	PHE	4.1
1	A	93	GLY	3.8
1	B	93	GLY	3.5
1	B	261	GLY	3.3
1	A	276	CYS	3.3
1	B	298	PHE	3.2
1	A	141	ILE	3.0
1	B	104	SER	2.9
1	A	15	TYR	2.8
1	B	185	ARG	2.7
1	A	32	VAL	2.7
1	A	253	GLY	2.7
1	B	122	GLU	2.6
1	B	205	CYS	2.5
1	B	276	CYS	2.5
1	B	179	HIS	2.5
1	A	143	GLY	2.4
1	B	88	ASN	2.3
1	B	17	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	50	ASP	2.2
1	A	302	THR	2.2
1	A	19	GLY	2.2
1	B	266	ASP	2.2
1	B	302	THR	2.2
1	A	140	ALA	2.2
1	A	299	ASP	2.2
1	B	22	LYS	2.2
1	A	235	ALA	2.2
1	A	7	SER	2.1
1	B	313	GLY	2.1
1	B	140	ALA	2.1
1	A	179	HIS	2.0
1	A	267	ASP	2.0
1	B	141	ILE	2.0
1	A	248	HIS	2.0
1	B	11	ARG	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 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
2	CS	B	405	1/1	0.15	0.29	27,27,27,27	1
2	CS	A	402	1/1	0.39	0.40	27,27,27,27	1
2	CS	A	401	1/1	0.78	0.10	27,27,27,27	1
2	CS	A	400	1/1	0.88	0.16	27,27,27,27	1
2	CS	B	404	1/1	0.89	0.24	27,27,27,27	1
2	CS	B	403	1/1	0.94	0.17	27,27,27,27	1

6.5 Other polymers [i](#)

There are no such residues in this entry.