



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 06:41 PM UTC

PDB ID : 4IX1 / pdb_00004ix1
Title : Crystal structure of hypothetical protein OPAG_01669 from Rhodococcus Opacus PD630, Target 016205
Authors : Malashkevich, V.N.; Bhosle, R.; Toro, R.; Hillerich, B.; Gizzi, A.; Garforth, S.; Kar, A.; Chan, M.K.; Laffuer, J.; Patel, H.; Matikainen, B.; Chamala, S.; Lim, S.; Celikgil, A.; Villegas, G.; Evans, B.; Zenchek, W.; Love, J.; Fiser, A.; Khafizov, K.; Seidel, R.; Bonanno, J.B.; Almo, S.C.; New York Structural Genomics Research Consortium (NYSGRG)
Deposited on : 2013-01-24
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
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)

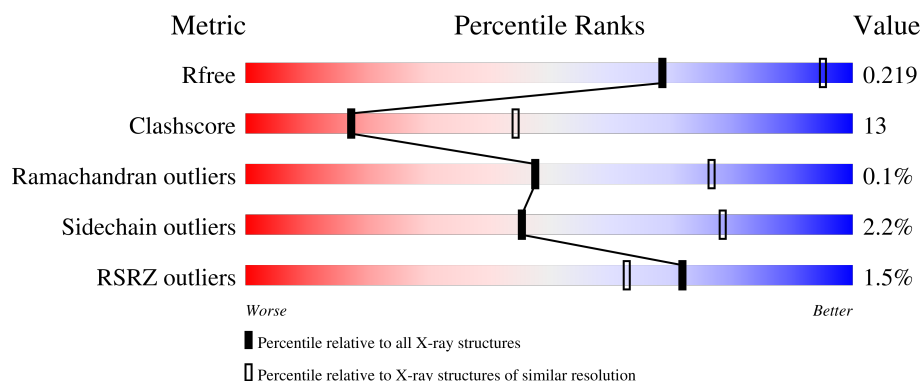
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

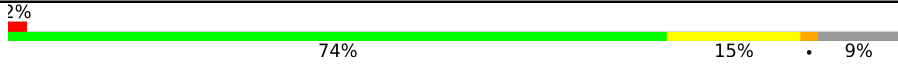
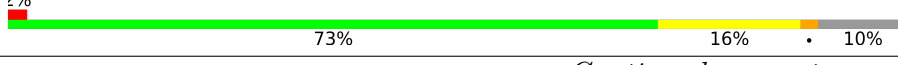
The reported resolution of this entry is 2.80 Å.

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	258	
1	B	258	
1	C	258	

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Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

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Mol	Chain	Length	Quality of chain
1	D	258	2% 73% 16% • 10%
1	E	258	% 71% 19% • 10%
1	F	258	75% 14% • 10%
1	G	258	74% 16% • 10%
1	H	258	% 70% 19% • 10%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 14075 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.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	234	Total	C	N	O	S	Se	0	0	0
			1752	1116	291	341	1	3			
1	B	234	Total	C	N	O	S	Se	0	1	0
			1757	1119	291	343	1	3			
1	C	233	Total	C	N	O	S	Se	0	0	0
			1747	1113	290	340	1	3			
1	D	233	Total	C	N	O	S	Se	0	0	0
			1747	1113	290	340	1	3			
1	E	233	Total	C	N	O	S	Se	0	0	0
			1747	1113	290	340	1	3			
1	F	232	Total	C	N	O	S	Se	0	0	0
			1742	1110	289	339	1	3			
1	G	233	Total	C	N	O	S	Se	0	0	0
			1747	1113	290	340	1	3			
1	H	233	Total	C	N	O	S	Se	0	0	0
			1747	1113	290	340	1	3			

- Molecule 2 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	P	0	0
			5	4	1		
2	D	1	Total	O	P	0	0
			5	4	1		

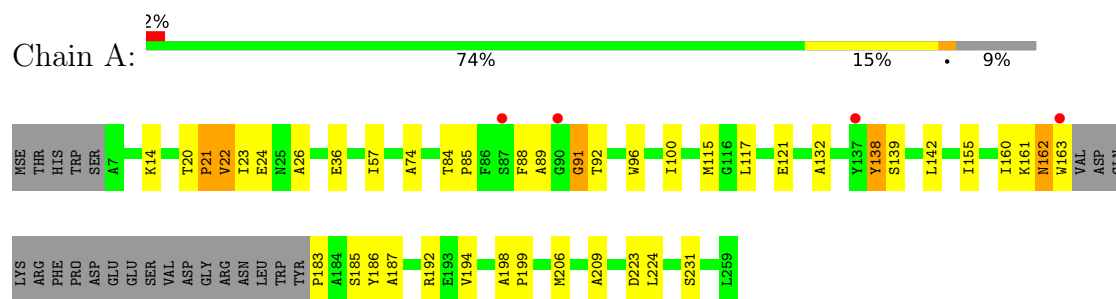
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	8	Total	O	0	0
			8	8		
3	B	13	Total	O	0	0
			13	13		
3	C	9	Total	O	0	0
			9	9		
3	D	9	Total	O	0	0
			9	9		
3	E	12	Total	O	0	0
			12	12		
3	F	9	Total	O	0	0
			9	9		
3	G	13	Total	O	0	0
			13	13		
3	H	6	Total	O	0	0
			6	6		

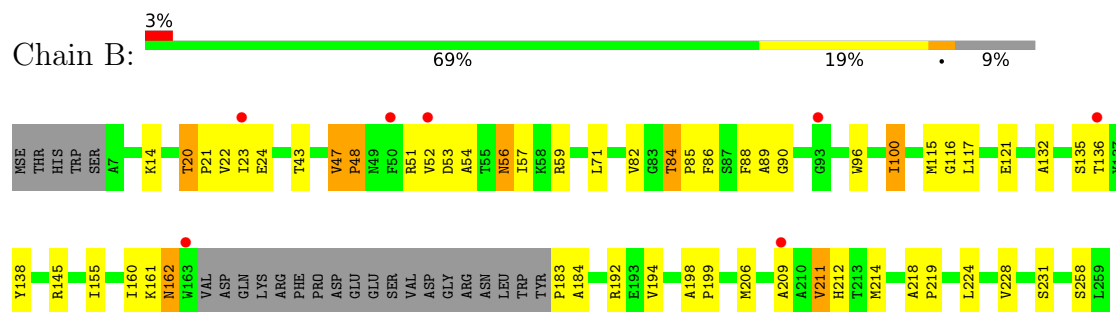
3 Residue-property plots

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.

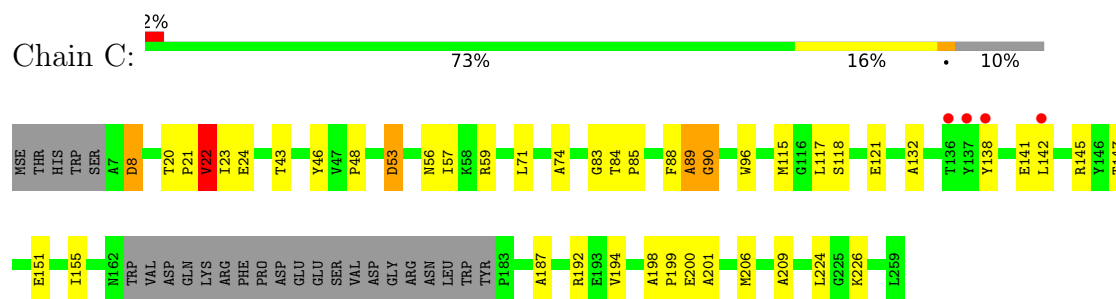
• Molecule 1: hypothetical protein



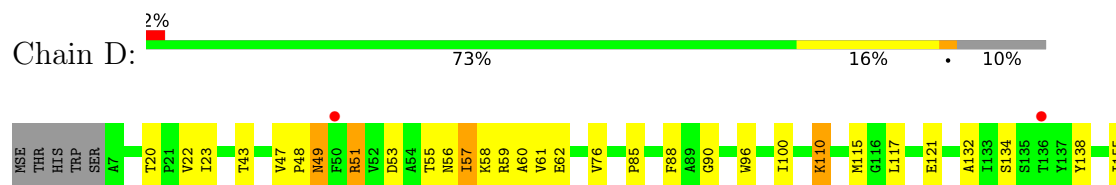
• Molecule 1: hypothetical protein

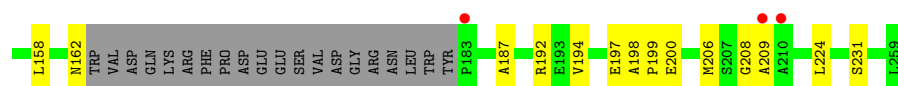


• Molecule 1: hypothetical protein

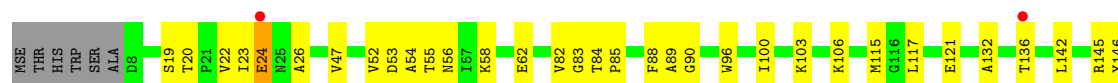


• Molecule 1: hypothetical protein





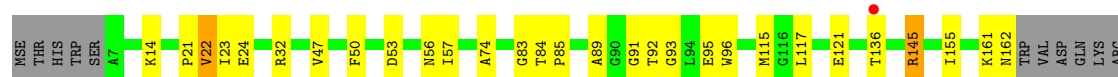
- Molecule 1: hypothetical protein



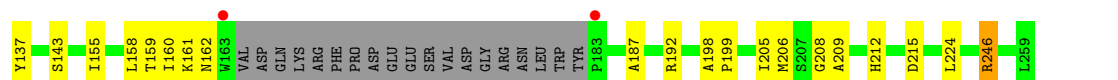
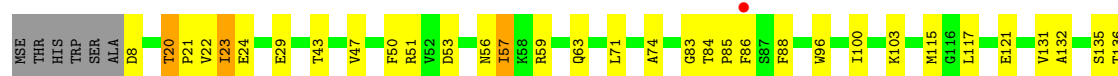
- Molecule 1: hypothetical protein



- Molecule 1: hypothetical protein



- Molecule 1: hypothetical protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	117.82Å 117.90Å 166.32Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.90 – 2.80 19.90 – 2.80	Depositor EDS
% Data completeness (in resolution range)	98.4 (19.90-2.80) 98.4 (19.90-2.80)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.38 (at 2.81Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.193 , 0.220 0.194 , 0.219	Depositor DCC
R_{free} test set	2897 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	71.5	Xtriage
Anisotropy	0.098	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 68.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.007 for k,h,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	14075	wwPDB-VP
Average B, all atoms (Å ²)	95.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.16% 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: PO4

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	3/1783 (0.2%)	1.08	7/2415 (0.3%)
1	B	1.10	6/1791 (0.3%)	1.12	14/2426 (0.6%)
1	C	1.03	2/1778 (0.1%)	1.04	6/2408 (0.2%)
1	D	1.02	2/1778 (0.1%)	1.05	6/2408 (0.2%)
1	E	1.08	3/1778 (0.2%)	1.12	9/2408 (0.4%)
1	F	0.98	2/1773 (0.1%)	1.07	6/2401 (0.2%)
1	G	0.97	2/1778 (0.1%)	1.01	2/2408 (0.1%)
1	H	0.99	2/1778 (0.1%)	1.08	5/2408 (0.2%)
All	All	1.03	22/14237 (0.2%)	1.07	55/19282 (0.3%)

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	G	0	1

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	21	PRO	N-CD	5.59	1.55	1.47
1	B	198	ALA	C-N	5.43	1.40	1.33
1	C	198	ALA	C-N	5.41	1.39	1.34
1	H	21	PRO	N-CD	5.35	1.55	1.47
1	E	199	PRO	N-CD	5.34	1.55	1.47
1	D	47	VAL	C-N	5.33	1.40	1.33
1	F	199	PRO	N-CD	5.32	1.55	1.47
1	C	199	PRO	N-CD	5.29	1.55	1.47
1	B	258	SER	CA-C	-5.28	1.45	1.52
1	D	199	PRO	N-CD	5.26	1.55	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	48	PRO	N-CD	5.19	1.55	1.47
1	H	199	PRO	N-CD	5.19	1.55	1.47
1	G	198	ALA	C-N	5.16	1.39	1.34
1	G	199	PRO	N-CD	5.16	1.54	1.47
1	B	84	THR	C-N	5.14	1.40	1.33
1	E	106	LYS	CA-CB	5.08	1.61	1.53
1	F	198	ALA	C-N	5.07	1.40	1.33
1	E	198	ALA	C-N	5.07	1.40	1.33
1	A	21	PRO	N-CD	5.06	1.54	1.47
1	A	199	PRO	N-CD	5.03	1.54	1.47
1	B	199	PRO	N-CD	5.03	1.54	1.47
1	A	198	ALA	C-N	5.02	1.39	1.34

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	90	GLY	N-CA-C	9.09	124.41	112.77
1	D	47	VAL	CA-C-N	-7.21	112.56	119.76
1	D	47	VAL	C-N-CA	-7.21	112.56	119.76
1	H	20	THR	CA-C-N	-6.88	112.61	121.91
1	H	20	THR	C-N-CA	-6.88	112.61	121.91
1	C	138	TYR	N-CA-C	6.77	119.69	110.55
1	D	90	GLY	N-CA-C	-6.76	97.16	113.18
1	E	103	LYS	CG-CD-CE	-6.55	96.22	111.30
1	E	52	VAL	N-CA-C	6.55	118.51	109.80
1	E	103	LYS	CD-CE-NZ	6.53	132.78	111.90
1	A	162	ASN	N-CA-C	-6.40	99.26	108.60
1	F	94	LEU	N-CA-C	6.36	118.29	111.36
1	G	198	ALA	CA-C-N	-6.22	113.40	119.87
1	G	198	ALA	C-N-CA	-6.22	113.40	119.87
1	H	198	ALA	CA-C-N	-6.08	113.55	119.87
1	H	198	ALA	C-N-CA	-6.08	113.55	119.87
1	C	198	ALA	CA-C-N	-6.01	113.93	119.82
1	C	198	ALA	C-N-CA	-6.01	113.93	119.82
1	A	198	ALA	CA-C-N	-5.99	113.64	119.87
1	A	198	ALA	C-N-CA	-5.99	113.64	119.87
1	F	89	ALA	N-CA-C	5.98	117.47	111.07
1	E	198	ALA	CA-C-N	-5.97	113.47	119.56
1	E	198	ALA	C-N-CA	-5.97	113.47	119.56
1	B	258	SER	CA-C-N	-5.76	111.34	121.70
1	B	258	SER	C-N-CA	-5.76	111.34	121.70
1	F	198	ALA	CA-C-N	-5.75	113.69	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	198	ALA	C-N-CA	-5.75	113.69	119.56
1	F	22	VAL	O-C-N	5.72	127.88	122.05
1	E	47	VAL	CA-C-N	-5.71	112.70	119.84
1	E	47	VAL	C-N-CA	-5.71	112.70	119.84
1	A	14	LYS	CG-CD-CE	-5.70	98.18	111.30
1	A	91	GLY	N-CA-C	5.70	121.77	110.77
1	B	211	VAL	N-CA-CB	5.68	118.04	110.26
1	A	138	TYR	N-CA-C	5.64	119.25	110.17
1	H	103	LYS	CA-CB-CG	5.51	125.13	114.10
1	B	211	VAL	CB-CA-C	-5.50	103.52	111.34
1	A	22	VAL	N-CA-C	-5.48	104.00	111.89
1	B	84	THR	CA-C-N	-5.44	113.29	119.28
1	B	84	THR	C-N-CA	-5.44	113.29	119.28
1	B	100	ILE	CG1-CB-CG2	-5.36	94.63	110.70
1	D	208	GLY	N-CA-C	-5.31	100.59	113.18
1	B	20	THR	CA-C-N	-5.31	113.20	119.84
1	B	20	THR	C-N-CA	-5.31	113.20	119.84
1	B	47	VAL	CA-C-N	-5.30	113.16	119.05
1	B	47	VAL	C-N-CA	-5.30	113.16	119.05
1	B	198	ALA	CA-C-N	-5.29	114.17	119.56
1	B	198	ALA	C-N-CA	-5.29	114.17	119.56
1	E	136	THR	N-CA-C	-5.27	105.53	111.28
1	B	54	ALA	N-CA-C	-5.21	105.49	111.07
1	D	198	ALA	CA-C-N	-5.18	113.58	119.28
1	D	198	ALA	C-N-CA	-5.18	113.58	119.28
1	F	22	VAL	N-CA-C	-5.18	107.30	111.91
1	C	89	ALA	CA-C-N	5.16	125.67	120.00
1	C	89	ALA	C-N-CA	5.16	125.67	120.00
1	E	54	ALA	N-CA-C	-5.04	105.78	111.28

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	G	249	SER	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	1752	0	1744	49	0
1	B	1757	0	1748	58	0
1	C	1747	0	1742	46	0
1	D	1747	0	1742	41	0
1	E	1747	0	1739	44	0
1	F	1742	0	1737	30	0
1	G	1747	0	1742	36	0
1	H	1747	0	1739	60	0
2	A	5	0	0	0	0
2	D	5	0	0	0	0
3	A	8	0	0	0	0
3	B	13	0	0	2	0
3	C	9	0	0	0	0
3	D	9	0	0	0	0
3	E	12	0	0	1	0
3	F	9	0	0	0	0
3	G	13	0	0	0	0
3	H	6	0	0	0	0
All	All	14075	0	13933	350	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 13.

All (350) 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:D:53:ASP:HB2	1:D:56:ASN:HB2	1.49	0.94
1:B:53:ASP:HB3	1:B:56:ASN:HB2	1.46	0.94
1:A:22:VAL:O	1:A:23:ILE:HG22	1.72	0.90
1:F:23:ILE:HG23	1:F:23:ILE:O	1.77	0.84
1:D:23:ILE:HG23	1:H:74:ALA:O	1.82	0.80
1:H:20:THR:OG1	1:H:22:VAL:HG22	1.82	0.79
1:C:21:PRO:C	1:C:23:ILE:H	1.90	0.78
1:E:20:THR:HG23	1:E:22:VAL:HG22	1.66	0.78
1:H:85:PRO:HA	1:H:88:PHE:CZ	2.19	0.77
1:C:22:VAL:HG12	1:C:24:GLU:HG2	1.67	0.76
1:H:131:VAL:HG11	1:H:205:ILE:HG13	1.68	0.76
1:G:145:ARG:HG3	1:G:145:ARG:HH21	1.52	0.75
1:H:212:HIS:NE2	1:H:215:ASP:OD2	2.20	0.75
1:G:53:ASP:OD1	1:G:56:ASN:HB2	1.86	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:20:THR:OG1	1:B:24:GLU:HG2	1.87	0.74
1:D:76:VAL:O	1:D:110:LYS:HD2	1.88	0.74
1:B:160:ILE:O	1:B:161:LYS:HD3	1.86	0.74
1:E:162:ASN:OD1	1:E:163:TRP:N	2.20	0.74
1:F:84:THR:HB	1:F:85:PRO:HD3	1.68	0.74
1:C:48:PRO:O	1:C:59:ARG:NH2	2.20	0.73
1:A:138:TYR:O	1:A:162:ASN:ND2	2.21	0.73
1:A:74:ALA:O	1:E:23:ILE:HG12	1.89	0.72
1:D:22:VAL:HG12	1:D:22:VAL:O	1.87	0.72
1:B:22:VAL:O	1:B:23:ILE:HG22	1.89	0.72
1:G:183:PRO:HG2	1:G:186:TYR:CD2	2.24	0.72
1:B:53:ASP:CB	1:B:56:ASN:HB2	2.20	0.72
1:B:183:PRO:HG2	1:B:184:ALA:H	1.55	0.71
1:B:162:ASN:N	1:B:162:ASN:HD22	1.88	0.71
1:B:53:ASP:O	1:B:57:ILE:HG13	1.91	0.70
1:C:20:THR:O	1:C:22:VAL:N	2.24	0.70
1:A:89:ALA:HB3	1:A:96:TRP:HE1	1.55	0.70
1:G:22:VAL:O	1:G:23:ILE:HG22	1.91	0.70
1:H:135:SER:O	1:H:162:ASN:CB	2.39	0.70
1:G:187:ALA:HB1	1:G:206:MSE:HE1	1.74	0.70
1:C:187:ALA:HB1	1:C:206:MSE:HE1	1.75	0.69
1:E:88:PHE:O	1:E:145:ARG:NH2	2.25	0.69
1:H:131:VAL:HG11	1:H:205:ILE:CG1	2.23	0.69
1:A:23:ILE:HG23	1:A:23:ILE:O	1.92	0.69
1:C:90:GLY:HA3	1:C:96:TRP:CD2	2.28	0.69
1:E:187:ALA:HB1	1:E:206:MSE:HE1	1.75	0.69
1:A:85:PRO:HA	1:A:88:PHE:CZ	2.27	0.68
1:A:85:PRO:HA	1:A:88:PHE:CE1	2.29	0.68
1:H:22:VAL:CG2	1:H:24:GLU:HG2	2.23	0.68
1:F:90:GLY:H	1:F:96:TRP:CD1	2.11	0.68
1:H:135:SER:O	1:H:162:ASN:HB3	1.94	0.68
1:H:136:THR:HG23	1:H:137:TYR:N	2.07	0.68
1:A:89:ALA:HB3	1:A:96:TRP:NE1	2.09	0.68
1:D:187:ALA:HB1	1:D:206:MSE:HE1	1.76	0.67
1:H:56:ASN:OD1	1:H:59:ARG:NH1	2.24	0.67
1:A:187:ALA:HB1	1:A:206:MSE:HE1	1.77	0.67
1:G:89:ALA:O	1:G:96:TRP:NE1	2.29	0.66
1:B:20:THR:OG1	1:B:22:VAL:HB	1.95	0.66
1:B:53:ASP:HB3	1:B:56:ASN:CB	2.24	0.66
1:D:51:ARG:O	1:D:56:ASN:ND2	2.28	0.66
1:E:20:THR:CG2	1:E:22:VAL:HG22	2.26	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:187:ALA:HB1	1:H:206:MSE:HE1	1.78	0.66
1:F:187:ALA:HB1	1:F:206:MSE:HE1	1.78	0.65
1:C:201:ALA:O	1:C:226:LYS:HE3	1.96	0.65
1:A:84:THR:HG23	1:A:85:PRO:HD3	1.78	0.65
1:E:201:ALA:O	1:E:226:LYS:HE3	1.96	0.65
1:C:56:ASN:OD1	1:C:59:ARG:NH1	2.30	0.65
1:A:91:GLY:O	1:A:92:THR:CG2	2.45	0.64
1:H:212:HIS:O	1:H:212:HIS:CD2	2.50	0.64
1:A:115:MSE:HE1	1:A:209:ALA:HB1	1.78	0.64
1:H:22:VAL:C	1:H:23:ILE:HG13	2.23	0.64
1:F:22:VAL:CG2	1:F:24:GLU:HB2	2.28	0.64
1:C:90:GLY:H	1:C:96:TRP:CD1	2.14	0.64
1:B:206:MSE:HE2	1:B:228:VAL:CG1	2.28	0.64
1:H:131:VAL:CG1	1:H:205:ILE:HG12	2.28	0.64
1:C:8:ASP:N	1:C:8:ASP:OD1	2.30	0.63
1:D:53:ASP:HB2	1:D:56:ASN:CB	2.26	0.63
1:H:22:VAL:HG22	1:H:24:GLU:HG2	1.79	0.63
1:C:23:ILE:HD11	1:G:14:LYS:HD3	1.81	0.62
1:C:53:ASP:C	1:C:53:ASP:OD1	2.41	0.62
1:H:29:GLU:OE2	1:H:212:HIS:ND1	2.33	0.61
1:H:23:ILE:HD12	1:H:23:ILE:O	2.00	0.61
1:D:115:MSE:HE2	1:D:209:ALA:HB2	1.83	0.61
1:H:53:ASP:O	1:H:57:ILE:HD12	2.02	0.60
1:D:22:VAL:O	1:D:23:ILE:HG12	2.01	0.60
1:C:115:MSE:HE3	1:C:209:ALA:HB2	1.84	0.60
1:E:23:ILE:O	1:E:23:ILE:HG22	2.00	0.60
1:B:23:ILE:HG23	1:B:23:ILE:O	2.01	0.60
1:C:21:PRO:C	1:C:23:ILE:N	2.50	0.60
1:C:23:ILE:HG23	1:C:23:ILE:O	2.01	0.60
1:C:22:VAL:O	1:C:23:ILE:HG22	2.02	0.59
1:D:23:ILE:O	1:D:23:ILE:HG13	2.01	0.59
1:D:115:MSE:HE1	1:D:209:ALA:HB1	1.84	0.59
1:H:115:MSE:CE	1:H:209:ALA:CB	2.80	0.59
1:F:23:ILE:O	1:F:23:ILE:CG2	2.47	0.59
1:A:115:MSE:CE	1:A:209:ALA:CB	2.81	0.59
1:D:51:ARG:C	1:D:56:ASN:HD22	2.09	0.59
1:G:115:MSE:HE3	1:G:209:ALA:HB2	1.84	0.58
1:C:90:GLY:H	1:C:96:TRP:NE1	2.01	0.58
1:G:115:MSE:CE	1:G:209:ALA:CB	2.81	0.58
1:H:159:THR:HG22	1:H:160:ILE:N	2.17	0.58
1:A:74:ALA:O	1:E:23:ILE:CG1	2.51	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:115:MSE:HE3	1:E:209:ALA:HB2	1.86	0.58
1:H:115:MSE:HE3	1:H:209:ALA:HB2	1.84	0.58
1:E:115:MSE:CE	1:E:209:ALA:CB	2.82	0.58
1:C:115:MSE:CE	1:C:209:ALA:CB	2.81	0.58
1:G:23:ILE:O	1:G:23:ILE:HG23	2.01	0.57
1:D:115:MSE:CE	1:D:209:ALA:CB	2.82	0.57
1:E:90:GLY:O	1:E:96:TRP:HB2	2.05	0.57
1:G:145:ARG:HH21	1:G:145:ARG:CG	2.15	0.57
1:H:135:SER:O	1:H:162:ASN:HB2	2.03	0.57
1:B:53:ASP:HB3	1:B:56:ASN:H	1.70	0.57
1:C:20:THR:C	1:C:22:VAL:H	2.13	0.57
1:F:22:VAL:HG23	1:F:24:GLU:HB2	1.86	0.56
1:F:22:VAL:O	1:F:23:ILE:HG22	2.04	0.56
1:E:20:THR:HG22	1:E:24:GLU:OE1	2.06	0.56
1:H:115:MSE:CE	1:H:209:ALA:HB2	2.36	0.56
1:H:115:MSE:HE1	1:H:209:ALA:CB	2.35	0.56
1:A:24:GLU:OE2	1:A:26:ALA:N	2.29	0.56
1:A:115:MSE:HE2	1:A:209:ALA:HB2	1.86	0.56
1:B:51:ARG:HG3	1:B:52:VAL:N	2.20	0.56
1:C:21:PRO:O	1:C:23:ILE:N	2.39	0.56
1:A:115:MSE:HE1	1:A:209:ALA:CB	2.36	0.56
1:B:135:SER:O	1:B:162:ASN:HB3	2.06	0.56
1:F:94:LEU:HD23	1:F:94:LEU:N	2.20	0.56
1:B:20:THR:HG1	1:B:22:VAL:HB	1.70	0.55
1:F:200:GLU:CD	1:F:200:GLU:H	2.15	0.55
1:H:136:THR:CG2	1:H:137:TYR:N	2.68	0.55
1:H:131:VAL:CG1	1:H:205:ILE:CG1	2.83	0.55
1:D:88:PHE:HD1	1:D:88:PHE:O	1.90	0.55
1:E:115:MSE:HE1	1:E:209:ALA:CB	2.37	0.55
1:C:22:VAL:HG12	1:C:24:GLU:CG	2.36	0.54
1:C:23:ILE:HB	1:G:74:ALA:O	2.07	0.54
1:C:115:MSE:CE	1:C:209:ALA:HB2	2.38	0.54
1:E:158:LEU:CD1	1:E:158:LEU:N	2.70	0.54
1:G:115:MSE:CE	1:G:209:ALA:HB2	2.37	0.54
1:G:115:MSE:HE1	1:G:209:ALA:CB	2.37	0.54
1:B:162:ASN:HD22	1:B:162:ASN:H	1.53	0.54
1:C:89:ALA:HB3	1:C:96:TRP:HE1	1.71	0.54
1:B:22:VAL:HG12	1:B:24:GLU:OE2	2.08	0.54
1:C:85:PRO:HA	1:C:88:PHE:CZ	2.43	0.54
1:D:22:VAL:O	1:D:23:ILE:CG1	2.56	0.54
1:H:158:LEU:CD1	1:H:158:LEU:N	2.71	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:90:GLY:O	1:B:96:TRP:HB2	2.08	0.53
1:E:115:MSE:CE	1:E:209:ALA:HB2	2.37	0.53
1:E:162:ASN:CG	1:E:163:TRP:N	2.66	0.53
1:C:115:MSE:HE1	1:C:209:ALA:CB	2.39	0.53
1:A:91:GLY:O	1:A:92:THR:HG22	2.08	0.53
1:B:138:TYR:O	1:B:162:ASN:OD1	2.26	0.53
1:B:14:LYS:HD3	1:F:23:ILE:HD11	1.89	0.53
1:E:146:TYR:OH	1:E:207:SER:OG	2.24	0.53
1:A:20:THR:C	1:A:22:VAL:H	2.15	0.53
1:C:84:THR:N	1:C:115:MSE:HE2	2.24	0.53
1:F:160:ILE:C	1:F:161:LYS:HG2	2.33	0.53
1:E:85:PRO:HA	1:E:88:PHE:CZ	2.44	0.53
1:D:96:TRP:CE2	1:D:100:ILE:HD11	2.44	0.53
1:B:48:PRO:HD2	1:B:59:ARG:HH12	1.74	0.52
1:H:96:TRP:CE2	1:H:100:ILE:HD11	2.45	0.52
1:B:115:MSE:HE1	1:B:209:ALA:CB	2.39	0.52
1:E:96:TRP:CE2	1:E:100:ILE:HD11	2.45	0.52
1:B:211:VAL:HG12	1:B:212:HIS:N	2.24	0.52
1:F:194:VAL:HA	1:F:197:GLU:HG2	1.92	0.52
1:A:84:THR:CG2	1:A:85:PRO:HD3	2.40	0.52
1:G:193:GLU:O	1:G:197:GLU:HG3	2.10	0.52
1:D:134:SER:OG	1:D:194:VAL:HG21	2.10	0.51
1:E:84:THR:N	1:E:115:MSE:HE2	2.25	0.51
1:A:74:ALA:C	1:E:23:ILE:HG12	2.34	0.51
1:C:74:ALA:O	1:G:23:ILE:HB	2.10	0.51
1:A:139:SER:H	1:A:142:LEU:HD12	1.75	0.51
1:C:141:GLU:HG3	1:C:142:LEU:N	2.24	0.51
1:D:48:PRO:O	1:D:49:ASN:HB2	2.11	0.51
1:A:192:ARG:HD2	1:A:224:LEU:HD21	1.93	0.51
1:F:194:VAL:HA	1:F:197:GLU:OE2	2.10	0.51
1:B:85:PRO:HG2	3:B:310:HOH:O	2.10	0.51
1:H:86:PHE:HE1	1:H:100:ILE:HD13	1.75	0.51
1:A:74:ALA:HB1	1:E:23:ILE:CD1	2.41	0.51
1:E:160:ILE:HG23	1:E:160:ILE:O	2.10	0.51
1:D:115:MSE:HE1	1:D:209:ALA:CB	2.41	0.50
1:H:86:PHE:CE1	1:H:100:ILE:HD13	2.47	0.50
1:A:96:TRP:CE2	1:A:100:ILE:HD11	2.46	0.50
1:C:20:THR:C	1:C:22:VAL:N	2.68	0.50
1:C:147:THR:O	1:C:151:GLU:HG3	2.10	0.50
1:E:20:THR:OG1	1:E:22:VAL:HG13	2.12	0.50
1:C:23:ILE:HD11	1:G:14:LYS:CD	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:84:THR:N	1:G:115:MSE:HE2	2.27	0.50
1:H:43:THR:HG22	1:H:71:LEU:HD11	1.93	0.50
1:H:84:THR:N	1:H:115:MSE:HE2	2.26	0.50
1:B:192:ARG:HD2	1:B:224:LEU:HD21	1.94	0.49
1:G:89:ALA:O	1:G:96:TRP:CE2	2.66	0.49
1:H:158:LEU:N	1:H:158:LEU:HD12	2.27	0.49
1:A:162:ASN:OD1	1:A:163:TRP:N	2.43	0.49
1:D:138:TYR:O	1:D:162:ASN:ND2	2.44	0.49
1:C:43:THR:HG22	1:C:71:LEU:HD11	1.95	0.49
1:F:192:ARG:HD2	1:F:224:LEU:HD21	1.94	0.49
1:E:158:LEU:N	1:E:158:LEU:HD12	2.26	0.48
1:D:22:VAL:O	1:D:22:VAL:CG1	2.57	0.48
1:G:192:ARG:HD2	1:G:224:LEU:HD21	1.95	0.48
1:H:85:PRO:HA	1:H:88:PHE:CE1	2.48	0.48
1:B:51:ARG:HG3	1:B:52:VAL:H	1.79	0.48
1:E:192:ARG:HD2	1:E:224:LEU:HD21	1.94	0.48
1:A:183:PRO:HG2	1:A:186:TYR:CD2	2.47	0.48
1:F:53:ASP:OD1	1:F:56:ASN:HB2	2.13	0.48
1:G:84:THR:N	1:G:85:PRO:HD2	2.29	0.48
1:D:192:ARG:HD2	1:D:224:LEU:HD21	1.96	0.47
1:H:117:LEU:O	1:H:121:GLU:HG3	2.14	0.47
1:D:85:PRO:HA	1:D:88:PHE:CZ	2.49	0.47
1:G:92:THR:O	1:G:95:GLU:OE2	2.33	0.47
1:A:91:GLY:O	1:A:92:THR:HG23	2.13	0.47
1:B:117:LEU:O	1:B:121:GLU:HG3	2.14	0.47
1:D:117:LEU:O	1:D:121:GLU:HG3	2.14	0.47
1:E:89:ALA:HB3	1:E:96:TRP:HE1	1.79	0.47
1:A:115:MSE:CE	1:A:209:ALA:HB2	2.44	0.47
1:H:131:VAL:HG12	1:H:132:ALA:N	2.29	0.47
1:H:159:THR:CG2	1:H:160:ILE:N	2.77	0.47
1:C:192:ARG:HD2	1:C:224:LEU:HD21	1.95	0.47
1:F:58:LYS:O	1:F:62:GLU:HG3	2.14	0.47
1:F:117:LEU:O	1:F:121:GLU:HG3	2.15	0.47
1:G:117:LEU:O	1:G:121:GLU:HG3	2.15	0.47
1:H:83:GLY:CA	1:H:115:MSE:HE2	2.44	0.47
1:B:20:THR:C	1:B:22:VAL:H	2.22	0.47
1:C:22:VAL:CG1	1:C:24:GLU:CD	2.88	0.47
1:E:84:THR:N	1:E:85:PRO:HD2	2.30	0.47
1:F:20:THR:C	1:F:22:VAL:H	2.21	0.47
1:H:22:VAL:O	1:H:23:ILE:HG13	2.15	0.47
1:B:183:PRO:CG	1:B:184:ALA:H	2.26	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:117:LEU:O	1:E:121:GLU:HG3	2.14	0.47
1:C:117:LEU:O	1:C:121:GLU:HG3	2.14	0.47
1:E:83:GLY:CA	1:E:115:MSE:HE2	2.45	0.47
1:H:192:ARG:HD2	1:H:224:LEU:HD21	1.96	0.47
1:A:22:VAL:O	1:A:23:ILE:CG2	2.55	0.47
1:H:143:SER:OG	1:H:162:ASN:ND2	2.48	0.46
1:A:117:LEU:O	1:A:121:GLU:HG3	2.14	0.46
1:G:136:THR:HA	1:G:162:ASN:HB3	1.98	0.46
1:A:23:ILE:O	1:A:23:ILE:CG2	2.60	0.46
1:B:84:THR:HG23	1:B:116:GLY:HA2	1.96	0.46
1:C:84:THR:H	1:C:115:MSE:HE2	1.81	0.46
1:H:160:ILE:O	1:H:161:LYS:HD3	2.15	0.46
1:D:23:ILE:HG23	1:H:74:ALA:C	2.38	0.46
1:B:51:ARG:HB3	1:B:56:ASN:OD1	2.15	0.46
1:G:83:GLY:CA	1:G:115:MSE:HE2	2.46	0.46
1:H:22:VAL:O	1:H:23:ILE:HD12	2.16	0.46
1:E:24:GLU:HG3	1:E:82:VAL:HG11	1.97	0.46
1:B:214:MSE:HG2	3:B:301:HOH:O	2.15	0.46
1:D:115:MSE:CE	1:D:209:ALA:HB2	2.43	0.46
1:A:162:ASN:CG	1:A:163:TRP:N	2.74	0.45
1:H:47:VAL:HG22	1:H:63:GLN:HG3	1.98	0.45
1:D:115:MSE:HE2	1:D:209:ALA:CB	2.45	0.45
1:G:89:ALA:O	1:G:96:TRP:CD1	2.69	0.45
1:H:162:ASN:OD1	1:H:162:ASN:O	2.33	0.45
1:C:83:GLY:CA	1:C:115:MSE:HE2	2.47	0.45
1:F:24:GLU:HG2	1:F:82:VAL:HG11	1.99	0.45
1:A:20:THR:C	1:A:22:VAL:N	2.75	0.45
1:B:211:VAL:CG1	1:B:212:HIS:N	2.80	0.45
1:B:96:TRP:O	1:B:100:ILE:HD13	2.16	0.45
1:B:136:THR:HA	1:B:162:ASN:HB2	1.98	0.45
1:F:94:LEU:O	1:F:95:GLU:C	2.59	0.45
1:B:20:THR:OG1	1:B:24:GLU:CG	2.61	0.45
1:E:90:GLY:O	1:E:96:TRP:CB	2.65	0.45
1:B:88:PHE:O	1:B:88:PHE:CD1	2.70	0.44
1:D:59:ARG:O	1:D:60:ALA:C	2.55	0.44
1:G:91:GLY:O	1:G:145:ARG:NH1	2.37	0.44
1:H:84:THR:N	1:H:85:PRO:HD2	2.32	0.44
1:A:160:ILE:O	1:A:161:LYS:HG2	2.17	0.44
1:B:89:ALA:H	1:B:96:TRP:CD1	2.35	0.44
1:G:145:ARG:CG	1:G:145:ARG:NH2	2.73	0.44
1:B:24:GLU:OE2	1:B:24:GLU:HA	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:135:SER:O	1:B:162:ASN:CB	2.65	0.44
1:H:22:VAL:HG23	1:H:24:GLU:HG2	1.98	0.44
1:A:91:GLY:C	1:A:92:THR:HG23	2.42	0.44
1:D:88:PHE:O	1:D:88:PHE:CD1	2.70	0.44
1:F:89:ALA:HB3	1:F:96:TRP:HE1	1.82	0.44
1:G:187:ALA:HB1	1:G:206:MSE:CE	2.46	0.44
1:B:206:MSE:HE2	1:B:228:VAL:HG11	1.99	0.44
1:C:187:ALA:HB1	1:C:206:MSE:CE	2.46	0.44
1:A:84:THR:HG23	1:A:85:PRO:CD	2.44	0.43
1:B:86:PHE:O	1:B:86:PHE:CD1	2.71	0.43
1:E:248:THR:OG1	3:E:301:HOH:O	2.21	0.43
1:B:135:SER:O	1:B:136:THR:C	2.60	0.43
1:B:183:PRO:HG2	1:B:184:ALA:N	2.28	0.43
1:G:21:PRO:C	1:G:23:ILE:N	2.74	0.43
1:B:43:THR:HG22	1:B:71:LEU:HD11	1.99	0.43
1:B:47:VAL:HG23	1:B:47:VAL:O	2.18	0.43
1:E:53:ASP:HB3	1:E:55:THR:OG1	2.18	0.43
1:D:22:VAL:C	1:D:23:ILE:HG12	2.44	0.43
1:D:158:LEU:CD1	1:D:158:LEU:N	2.80	0.43
1:C:84:THR:N	1:C:85:PRO:HD2	2.34	0.43
1:B:145:ARG:NH1	1:B:145:ARG:HG3	2.34	0.43
1:D:132:ALA:HB1	1:D:194:VAL:CG1	2.49	0.43
1:G:32:ARG:O	1:G:249:SER:OG	2.32	0.43
1:H:137:TYR:HB3	1:H:208:GLY:HA3	1.99	0.43
1:B:53:ASP:N	1:B:56:ASN:HB2	2.34	0.43
1:B:88:PHE:O	1:B:88:PHE:HD1	2.01	0.43
1:B:206:MSE:HE2	1:B:228:VAL:HG12	1.99	0.43
1:E:24:GLU:HG2	1:E:26:ALA:H	1.83	0.43
1:C:132:ALA:HB1	1:C:194:VAL:CG1	2.49	0.42
1:D:187:ALA:HB1	1:D:206:MSE:CE	2.48	0.42
1:A:115:MSE:HE2	1:A:231:SER:CB	2.50	0.42
1:E:90:GLY:O	1:E:96:TRP:CG	2.72	0.42
1:A:84:THR:CG2	1:A:85:PRO:CD	2.98	0.42
1:D:158:LEU:N	1:D:158:LEU:HD12	2.34	0.42
1:B:115:MSE:HE3	1:B:231:SER:HB3	2.01	0.42
1:C:22:VAL:CG1	1:C:24:GLU:HG2	2.44	0.42
1:H:84:THR:H	1:H:115:MSE:HE2	1.84	0.42
1:E:84:THR:H	1:E:115:MSE:HE2	1.85	0.42
1:E:187:ALA:HB1	1:E:206:MSE:CE	2.47	0.42
1:G:248:THR:HG21	1:G:256:LEU:HB3	2.01	0.42
1:H:29:GLU:OE2	1:H:212:HIS:CE1	2.72	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:223:ASP:HA	1:H:246:ARG:HG3	2.01	0.42
1:F:20:THR:O	1:F:22:VAL:N	2.46	0.42
1:G:84:THR:H	1:G:115:MSE:HE2	1.85	0.42
1:H:131:VAL:HG13	1:H:205:ILE:HG12	2.02	0.41
1:E:132:ALA:HB1	1:E:194:VAL:CG1	2.50	0.41
1:B:132:ALA:HB1	1:B:194:VAL:CG1	2.50	0.41
1:H:50:PHE:O	1:H:51:ARG:HG3	2.20	0.41
1:A:115:MSE:CE	1:A:231:SER:CB	2.99	0.41
1:A:115:MSE:HE2	1:A:231:SER:HB3	2.02	0.41
1:A:187:ALA:HB1	1:A:206:MSE:CE	2.48	0.41
1:B:48:PRO:HD2	1:B:59:ARG:NH1	2.34	0.41
1:F:57:ILE:HD13	1:F:57:ILE:HA	1.96	0.41
1:F:218:ALA:HB3	1:F:219:PRO:HD3	2.03	0.41
1:G:47:VAL:HG12	1:G:50:PHE:HB2	2.02	0.41
1:A:21:PRO:C	1:A:23:ILE:N	2.77	0.41
1:A:91:GLY:C	1:A:92:THR:CG2	2.94	0.41
1:C:200:GLU:OE1	1:C:200:GLU:N	2.52	0.41
1:G:93:GLY:HA3	1:G:95:GLU:OE1	2.20	0.41
1:A:132:ALA:HB1	1:A:194:VAL:CG1	2.51	0.41
1:D:200:GLU:H	1:D:200:GLU:CD	2.28	0.41
1:F:140:ARG:O	1:F:141:GLU:C	2.64	0.41
1:A:115:MSE:CE	1:A:209:ALA:HB1	2.45	0.41
1:D:115:MSE:CE	1:D:231:SER:CB	2.99	0.41
1:C:46:TYR:CZ	1:C:48:PRO:HG3	2.55	0.41
1:D:43:THR:HA	1:H:43:THR:HA	2.03	0.41
1:E:19:SER:HA	1:E:24:GLU:OE1	2.19	0.41
1:E:53:ASP:HB2	1:E:56:ASN:ND2	2.36	0.41
1:F:94:LEU:O	1:F:96:TRP:N	2.53	0.41
1:F:132:ALA:HB1	1:F:194:VAL:CG1	2.50	0.41
1:G:161:LYS:HE2	1:G:197:GLU:OE2	2.20	0.41
1:H:47:VAL:HG12	1:H:50:PHE:HB2	2.02	0.41
1:E:20:THR:C	1:E:22:VAL:H	2.29	0.41
1:F:20:THR:HA	1:F:21:PRO:HD3	1.89	0.41
1:B:53:ASP:HB3	1:B:56:ASN:N	2.36	0.40
1:B:218:ALA:HB3	1:B:219:PRO:HD3	2.03	0.40
1:C:88:PHE:O	1:C:145:ARG:NH2	2.54	0.40
1:C:89:ALA:HB3	1:C:96:TRP:NE1	2.35	0.40
1:E:58:LYS:O	1:E:62:GLU:HG3	2.20	0.40
1:H:20:THR:C	1:H:22:VAL:H	2.30	0.40
1:H:22:VAL:HG22	1:H:24:GLU:CG	2.50	0.40
1:A:115:MSE:HE2	1:A:209:ALA:CB	2.48	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:61:VAL:O	1:F:65:GLU:HG3	2.21	0.40
1:D:58:LYS:O	1:D:62:GLU:HG3	2.21	0.40
1:A:185:SER:OG	1:H:8:ASP:OD2	2.39	0.40
1:D:20:THR:C	1:D:22:VAL:H	2.30	0.40
1:D:57:ILE:O	1:D:61:VAL:HG23	2.22	0.40
1:D:115:MSE:CE	1:D:231:SER:HB3	2.51	0.40
1:B:24:GLU:HG3	1:B:82:VAL:HG11	2.03	0.40
1:B:162:ASN:N	1:B:162:ASN:ND2	2.60	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	230/258 (89%)	223 (97%)	7 (3%)	0	100	100
1	B	231/258 (90%)	221 (96%)	10 (4%)	0	100	100
1	C	229/258 (89%)	221 (96%)	7 (3%)	1 (0%)	30	60
1	D	229/258 (89%)	222 (97%)	6 (3%)	1 (0%)	30	60
1	E	229/258 (89%)	222 (97%)	7 (3%)	0	100	100
1	F	228/258 (88%)	219 (96%)	9 (4%)	0	100	100
1	G	229/258 (89%)	222 (97%)	7 (3%)	0	100	100
1	H	229/258 (89%)	222 (97%)	7 (3%)	0	100	100
All	All	1834/2064 (89%)	1772 (97%)	60 (3%)	2 (0%)	48	77

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	22	VAL
1	D	49	ASN

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	181/201 (90%)	178 (98%)	3 (2%)	53	83
1	B	182/201 (90%)	179 (98%)	3 (2%)	55	83
1	C	181/201 (90%)	175 (97%)	6 (3%)	33	69
1	D	181/201 (90%)	175 (97%)	6 (3%)	33	69
1	E	181/201 (90%)	178 (98%)	3 (2%)	53	83
1	F	181/201 (90%)	179 (99%)	2 (1%)	65	87
1	G	181/201 (90%)	176 (97%)	5 (3%)	38	73
1	H	181/201 (90%)	177 (98%)	4 (2%)	45	78
All	All	1449/1608 (90%)	1417 (98%)	32 (2%)	45	78

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	GLU
1	A	57	ILE
1	A	155	ILE
1	B	56	ASN
1	B	155	ILE
1	B	162	ASN
1	C	8	ASP
1	C	22	VAL
1	C	53	ASP
1	C	57	ILE
1	C	118	SER
1	C	155	ILE
1	D	51	ARG
1	D	55	THR
1	D	57	ILE
1	D	110	LYS
1	D	155	ILE
1	D	197	GLU
1	E	24	GLU

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Mol	Chain	Res	Type
1	E	142	LEU
1	E	155	ILE
1	F	53	ASP
1	F	155	ILE
1	G	22	VAL
1	G	24	GLU
1	G	57	ILE
1	G	145	ARG
1	G	155	ILE
1	H	23	ILE
1	H	57	ILE
1	H	155	ILE
1	H	246	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	81	GLN
1	B	162	ASN
1	C	25	ASN
1	C	81	GLN
1	D	56	ASN
1	D	162	ASN
1	F	25	ASN
1	F	81	GLN
1	H	25	ASN
1	H	63	GLN
1	H	81	GLN
1	H	162	ASN

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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

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	$\# Z > 2$
2	PO4	A	301	-	4,4,4	0.64	0	6,6,6	1.14	0
2	PO4	D	301	-	4,4,4	0.81	0	6,6,6	0.85	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [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	231/258 (89%)	-0.30	4 (1%) 69 60	56, 83, 150, 190	0
1	B	231/258 (89%)	-0.24	7 (3%) 52 42	56, 82, 155, 191	1 (0%)
1	C	230/258 (89%)	-0.26	4 (1%) 69 60	57, 82, 141, 169	0
1	D	230/258 (89%)	-0.18	5 (2%) 62 52	52, 96, 166, 212	0
1	E	230/258 (89%)	-0.27	3 (1%) 75 66	55, 78, 138, 178	0
1	F	229/258 (88%)	-0.23	1 (0%) 88 84	56, 91, 150, 178	0
1	G	230/258 (89%)	-0.35	1 (0%) 88 84	57, 84, 147, 181	0
1	H	230/258 (89%)	-0.22	3 (1%) 75 66	57, 95, 162, 183	0
All	All	1841/2064 (89%)	-0.25	28 (1%) 72 63	52, 86, 153, 212	1 (0%)

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	136	THR	5.0
1	B	52	VAL	3.4
1	G	136	THR	3.3
1	H	163	TRP	3.3
1	C	136	THR	3.3
1	D	136	THR	3.0
1	B	50	PHE	2.6
1	B	209	ALA	2.6
1	D	209	ALA	2.5
1	D	210	ALA	2.5
1	B	93	GLY	2.5
1	A	163	TRP	2.4
1	C	137	TYR	2.4
1	A	87	SER	2.4
1	H	183	PRO	2.4
1	B	23	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	H	86	PHE	2.3
1	B	163	TRP	2.3
1	D	50	PHE	2.2
1	D	183	PRO	2.2
1	A	90	GLY	2.2
1	E	183	PRO	2.2
1	B	136	THR	2.2
1	F	93	GLY	2.2
1	E	24	GLU	2.1
1	C	138	TYR	2.1
1	C	142	LEU	2.1
1	A	137	TYR	2.1

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

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

6.3 Carbohydrates [i](#)

There are no 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	PO4	A	301	5/5	0.89	0.13	119,127,131,138	0
2	PO4	D	301	5/5	0.97	0.06	117,122,131,134	0

6.5 Other polymers [i](#)

There are no such residues in this entry.