



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 11:33 AM UTC

PDB ID : 8YRE / pdb_00008yre
Title : Crystal structure of Arabidopsis VTC1-KJC2
Authors : Zhang, C.; Liu, L.
Deposited on : 2024-03-21
Resolution : 3.54 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

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

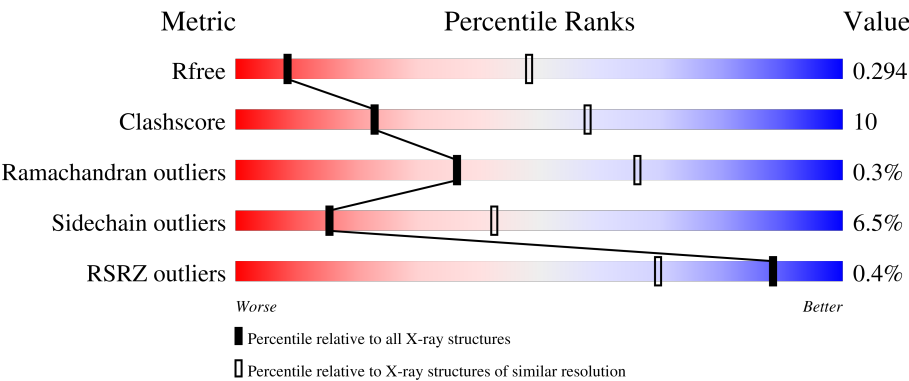
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.54 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	1008 (3.58-3.50)
Clashscore	190562	1062 (3.58-3.50)
Ramachandran outliers	187476	1033 (3.58-3.50)
Sidechain outliers	187428	1034 (3.58-3.50)
RSRZ outliers	180081	1007 (3.58-3.50)

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	406	62%31%• 5%
1	B	406	65%27%• 5%
1	C	406	% 67%24%• 6%
2	D	361	75%23%•
2	E	361	% 75%22%••

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Mol	Chain	Length	Quality of chain
2	F	361	73% 23% ••

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 17197 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.

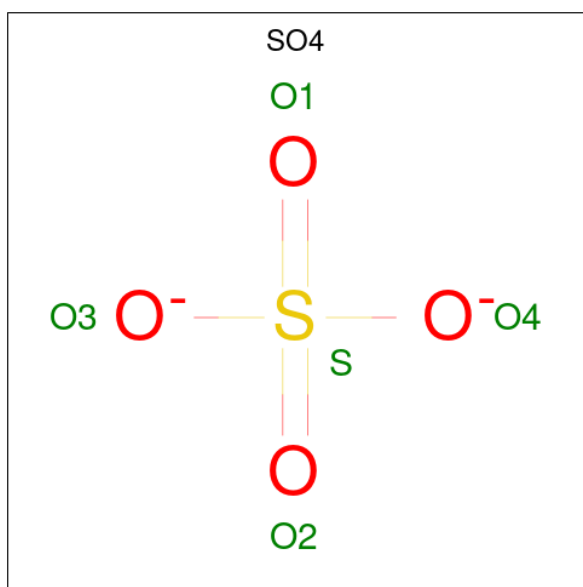
- Molecule 1 is a protein called ADP-glucose pyrophosphorylase family protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	387	Total	C	N	O	S	0	0	0
			2989	1920	506	552	11			
1	B	387	Total	C	N	O	S	0	0	0
			2989	1920	506	552	11			
1	C	381	Total	C	N	O	S	0	0	0
			2919	1870	500	541	8			

- Molecule 2 is a protein called Mannose-1-phosphate guanylyltransferase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	361	Total	C	N	O	S	0	0	0
			2771	1782	463	510	16			
2	E	359	Total	C	N	O	S	0	0	0
			2744	1764	461	504	15			
2	F	355	Total	C	N	O	S	0	0	0
			2723	1750	457	500	16			

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total	O	S	0	0
			5	4	1		
3	F	1	Total	O	S	0	0
			5	4	1		
3	F	1	Total	O	S	0	0
			5	4	1		

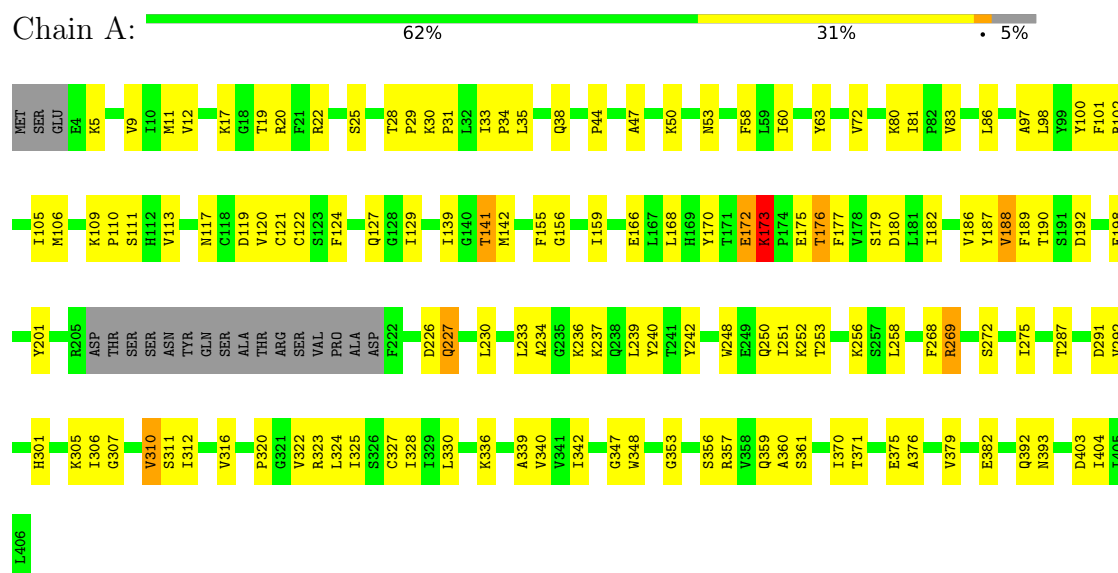
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total 1	O 1	0	0
4	B	1	Total 1	O 1	0	0

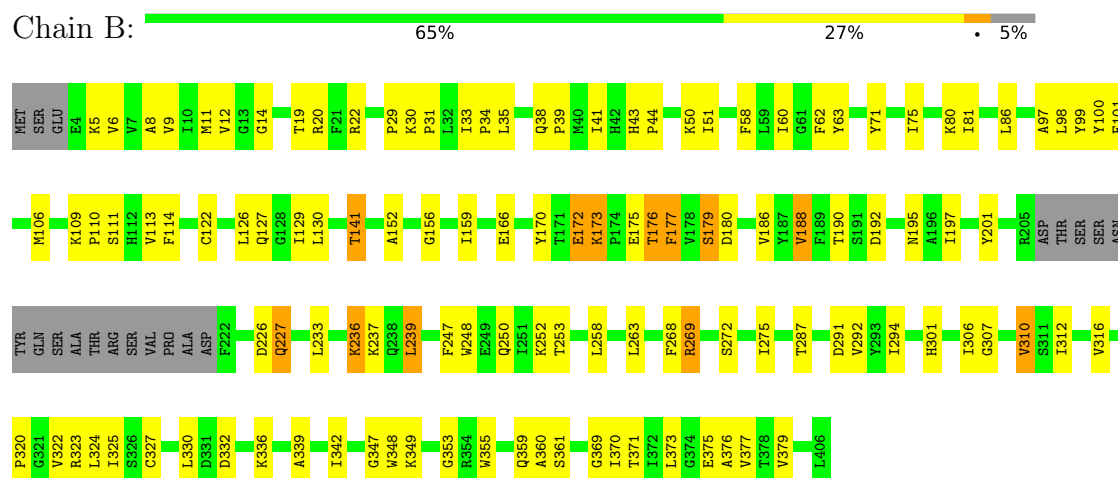
3 Residue-property plots

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: ADP-glucose pyrophosphorylase family protein

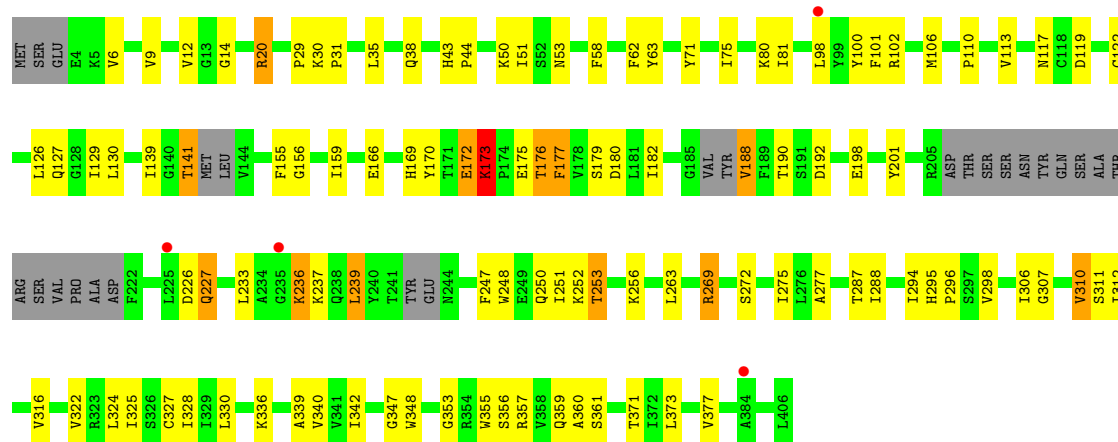


- Molecule 1: ADP-glucose pyrophosphorylase family protein



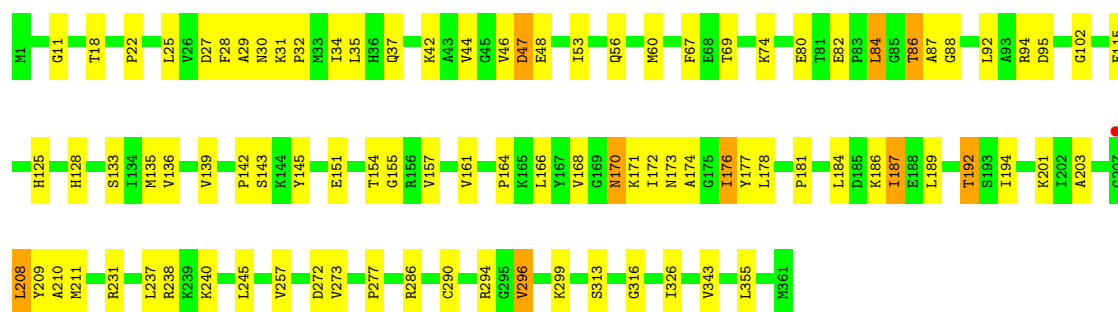
- Molecule 1: ADP-glucose pyrophosphorylase family protein





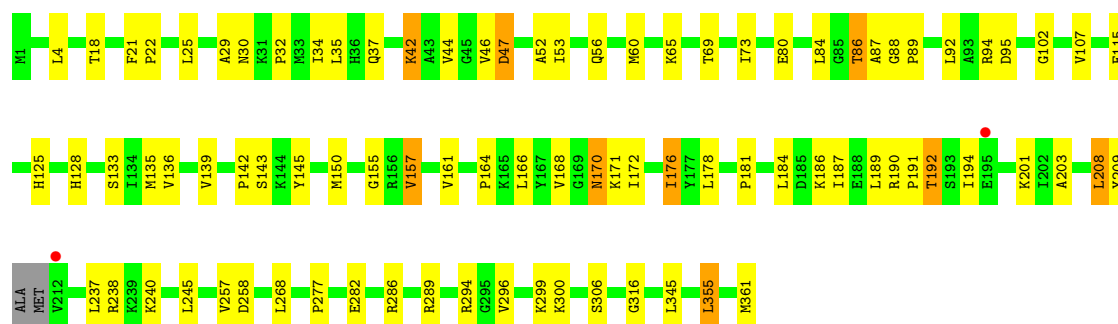
• Molecule 2: Mannose-1-phosphate guanylyltransferase 1

Chain D: 75% 23%



• Molecule 2: Mannose-1-phosphate guanylyltransferase 1

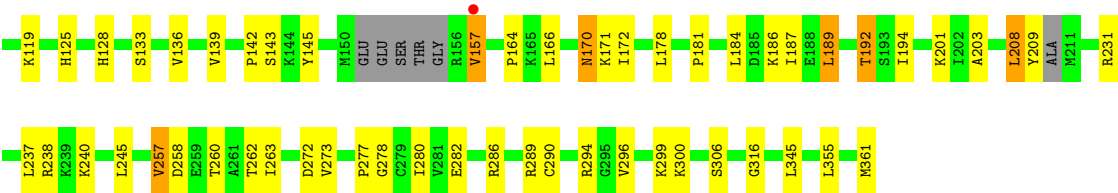
Chain E: 75% 22%



• Molecule 2: Mannose-1-phosphate guanylyltransferase 1

Chain F: 73% 23%





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	158.27Å 134.99Å 168.47Å 90.00° 117.14° 90.00°	Depositor
Resolution (Å)	149.92 – 3.54 149.92 – 3.54	Depositor EDS
% Data completeness (in resolution range)	96.3 (149.92-3.54) 92.5 (149.92-3.54)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.44 (at 3.58Å)	Xtriage
Refinement program	PHENIX 1.18	Depositor
R, R_{free}	0.261 , 0.295 0.261 , 0.294	Depositor DCC
R_{free} test set	1918 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	94.4	Xtriage
Anisotropy	0.503	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 252.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.105 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	17197	wwPDB-VP
Average B, all atoms (Å ²)	136.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.69% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4

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	0.13	0/3052	0.33	0/4145
1	B	0.14	0/3052	0.35	0/4145
1	C	0.13	0/2977	0.33	0/4039
2	D	0.15	0/2826	0.32	0/3826
2	E	0.11	0/2797	0.31	0/3787
2	F	0.11	0/2775	0.31	0/3754
All	All	0.13	0/17479	0.33	0/23696

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2989	0	3017	79	0
1	B	2989	0	3017	66	0
1	C	2919	0	2918	62	0
2	D	2771	0	2870	53	0
2	E	2744	0	2840	51	0
2	F	2723	0	2815	51	0
3	A	15	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	5	0	0	0	0
3	D	20	0	0	0	0
3	E	10	0	0	0	0
3	F	10	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
All	All	17197	0	17477	359	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (359) 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)
2:D:133:SER:HB3	2:D:178:LEU:HB3	1.59	0.84
2:D:84:LEU:HB2	2:D:88:GLY:HA3	1.60	0.83
2:E:133:SER:HB3	2:E:178:LEU:HB3	1.64	0.80
1:A:307:GLY:HA3	1:A:325:ILE:HG22	1.65	0.77
1:C:50:LYS:HE2	1:C:127:GLN:H	1.51	0.74
1:C:307:GLY:HA3	1:C:325:ILE:HG22	1.69	0.74
1:B:348:TRP:HB2	1:B:375:GLU:HG3	1.70	0.73
1:A:226:ASP:OD1	1:A:227:GLN:NE2	2.22	0.72
2:E:86:THR:HB	2:E:194:ILE:H	1.55	0.70
2:E:115:GLU:HB3	2:E:240:LYS:HZ1	1.57	0.69
1:B:307:GLY:HA3	1:B:325:ILE:HG22	1.76	0.68
2:E:34:ILE:O	2:E:37:GLN:NE2	2.26	0.67
1:B:35:LEU:N	1:B:38:GLN:O	2.26	0.67
2:E:125:HIS:ND1	2:E:209:TYR:OH	2.25	0.67
1:A:348:TRP:HB2	1:A:375:GLU:HG3	1.77	0.66
2:D:135:MET:HB2	2:D:176:ILE:HG23	1.77	0.66
1:A:348:TRP:O	1:A:376:ALA:N	2.26	0.66
2:D:34:ILE:O	2:D:37:GLN:NE2	2.29	0.66
2:F:133:SER:HB3	2:F:178:LEU:HB3	1.78	0.66
1:A:12:VAL:HG13	1:A:31:PRO:HG2	1.79	0.66
2:E:94:ARG:NH2	2:E:184:LEU:O	2.29	0.65
1:B:269:ARG:HH21	1:B:291:ASP:H	1.44	0.65
2:E:299:LYS:HD2	2:E:316:GLY:HA2	1.78	0.65
2:E:47:ASP:N	2:E:47:ASP:OD1	2.30	0.64
1:A:382:GLU:OE2	2:D:286:ARG:NE	2.29	0.63
1:C:340:VAL:HB	1:C:357:ARG:HG3	1.80	0.63
2:D:86:THR:HB	2:D:194:ILE:H	1.61	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:203:ALA:HA	2:F:208:LEU:HD11	1.79	0.63
2:F:84:LEU:HB2	2:F:88:GLY:HA3	1.80	0.63
2:D:277:PRO:HD2	2:D:294:ARG:HG2	1.80	0.62
2:F:142:PRO:HB3	2:F:170:ASN:HA	1.80	0.62
2:F:299:LYS:HD2	2:F:316:GLY:HA2	1.81	0.62
1:B:50:LYS:HE2	1:B:127:GLN:H	1.62	0.62
1:B:11:MET:HE1	1:B:97:ALA:HB3	1.82	0.62
1:A:122:CYS:HB3	1:A:248:TRP:HD1	1.65	0.62
1:B:348:TRP:O	1:B:376:ALA:N	2.28	0.61
1:C:306:ILE:HG22	1:C:310:VAL:HG11	1.82	0.61
1:A:159:ILE:HD13	1:A:179:SER:HB2	1.82	0.61
1:B:306:ILE:HG22	1:B:310:VAL:HG11	1.82	0.61
2:D:299:LYS:HD2	2:D:316:GLY:HA2	1.83	0.61
2:F:86:THR:HB	2:F:194:ILE:H	1.66	0.61
1:A:306:ILE:HG22	1:A:310:VAL:HG11	1.81	0.61
2:E:102:GLY:HA2	2:E:181:PRO:HG2	1.83	0.60
2:D:186:LYS:HZ2	2:D:201:LYS:HD3	1.65	0.60
2:F:94:ARG:NH2	2:F:184:LEU:O	2.34	0.60
2:F:47:ASP:OD1	2:F:47:ASP:N	2.35	0.60
2:E:135:MET:HB2	2:E:176:ILE:HG23	1.84	0.59
2:F:237:LEU:HB3	2:F:245:LEU:HD11	1.84	0.59
2:D:125:HIS:ND1	2:D:209:TYR:OH	2.26	0.59
2:F:143:SER:HA	2:F:164:PRO:HD2	1.85	0.59
1:A:156:GLY:HA2	1:A:175:GLU:HB3	1.85	0.59
1:A:9:VAL:HG22	1:A:58:PHE:HB2	1.84	0.59
1:A:35:LEU:N	1:A:38:GLN:O	2.36	0.58
1:B:330:LEU:HD12	1:B:347:GLY:HA2	1.84	0.58
2:D:115:GLU:HB3	2:D:240:LYS:HZ1	1.68	0.58
2:D:155:GLY:O	2:D:210:ALA:N	2.36	0.58
2:F:277:PRO:HD2	2:F:294:ARG:HG2	1.84	0.58
1:B:360:ALA:HB2	1:B:371:THR:HG22	1.85	0.58
1:B:156:GLY:HA2	1:B:175:GLU:HB3	1.86	0.58
2:D:47:ASP:OD1	2:D:47:ASP:N	2.37	0.58
2:E:237:LEU:HB3	2:E:245:LEU:HD11	1.85	0.58
2:D:80:GLU:HG3	2:D:92:LEU:HD13	1.86	0.57
2:E:84:LEU:HB2	2:E:88:GLY:HA3	1.85	0.57
1:B:294:ILE:HG12	1:B:312:ILE:HD12	1.86	0.57
2:E:190:ARG:CZ	2:E:191:PRO:HD2	2.35	0.57
1:C:12:VAL:HG13	1:C:31:PRO:HG2	1.87	0.57
1:B:336:LYS:HD2	1:B:353:GLY:HA2	1.86	0.56
2:D:44:VAL:HG23	2:D:46:VAL:HG23	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:5:LYS:O	1:A:111:SER:N	2.37	0.56
2:E:186:LYS:HZ2	2:E:201:LYS:HD3	1.71	0.56
1:A:330:LEU:HD12	1:A:347:GLY:HA2	1.88	0.56
1:C:29:PRO:HB3	1:C:63:TYR:CZ	2.41	0.56
2:F:80:GLU:HG3	2:F:92:LEU:HD13	1.86	0.56
1:A:190:THR:HG23	1:A:192:ASP:H	1.70	0.56
1:B:190:THR:HG23	1:B:192:ASP:H	1.71	0.56
2:E:142:PRO:HB3	2:E:170:ASN:HA	1.86	0.55
2:E:143:SER:HA	2:E:164:PRO:HD2	1.88	0.55
1:B:6:VAL:HG21	1:B:130:LEU:HD11	1.89	0.55
1:C:35:LEU:N	1:C:38:GLN:O	2.39	0.55
2:F:115:GLU:HB3	2:F:240:LYS:HZ1	1.71	0.55
1:A:258:LEU:HD12	1:A:370:ILE:HD12	1.87	0.55
1:C:6:VAL:HG21	1:C:130:LEU:HD11	1.89	0.54
2:D:133:SER:HB2	2:D:209:TYR:CZ	2.41	0.54
1:C:322:VAL:HG12	1:C:339:ALA:H	1.73	0.54
2:F:139:VAL:HG21	2:F:145:TYR:HD2	1.72	0.54
1:C:20:ARG:HH21	1:C:253:THR:HG23	1.72	0.54
1:C:336:LYS:HD2	1:C:353:GLY:HA2	1.90	0.54
1:B:170:TYR:OH	1:B:226:ASP:HB2	2.08	0.54
1:A:172:GLU:HG2	1:A:227:GLN:HG3	1.90	0.53
1:A:120:VAL:HG13	1:A:248:TRP:HE1	1.72	0.53
1:A:139:ILE:HG22	1:A:189:PHE:HD1	1.72	0.53
1:B:159:ILE:HD13	1:B:179:SER:HB2	1.91	0.53
1:C:129:ILE:HD11	1:C:141:THR:HB	1.91	0.53
2:D:133:SER:O	2:D:178:LEU:N	2.41	0.53
1:B:330:LEU:HD13	1:B:348:TRP:CE2	2.43	0.53
1:C:102:ARG:NH1	1:C:198:GLU:OE2	2.42	0.53
1:C:190:THR:HG23	1:C:192:ASP:H	1.74	0.53
1:A:330:LEU:HD13	1:A:348:TRP:CE2	2.45	0.53
1:C:122:CYS:HB3	1:C:248:TRP:HD1	1.73	0.53
2:E:133:SER:HB2	2:E:209:TYR:CZ	2.44	0.53
1:A:170:TYR:OH	1:A:226:ASP:HB2	2.09	0.52
1:B:355:TRP:CE2	2:E:286:ARG:HB2	2.45	0.52
1:B:106:MET:SD	1:B:110:PRO:HD2	2.48	0.52
1:A:292:VAL:HG13	1:A:310:VAL:HG13	1.91	0.52
2:F:102:GLY:HA2	2:F:181:PRO:HG2	1.91	0.52
1:A:375:GLU:HB3	1:A:392:GLN:HB2	1.92	0.52
1:A:117:ASN:ND2	1:A:119:ASP:OD1	2.43	0.52
2:D:34:ILE:HA	2:D:37:GLN:HE22	1.75	0.51
2:E:150:MET:HE3	2:E:155:GLY:HA2	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:277:PRO:HD2	2:E:294:ARG:HG2	1.92	0.51
1:A:141:THR:HG22	1:A:240:TYR:HB2	1.91	0.51
1:C:172:GLU:HG2	1:C:227:GLN:HG3	1.92	0.51
1:A:311:SER:HB2	1:A:328:ILE:HG22	1.92	0.51
1:C:330:LEU:HD12	1:C:347:GLY:HA2	1.92	0.51
2:D:143:SER:HA	2:D:164:PRO:HD2	1.93	0.51
2:F:260:THR:HB	2:F:278:GLY:H	1.76	0.51
1:B:12:VAL:HG13	1:B:31:PRO:HG2	1.92	0.51
1:B:353:GLY:N	1:B:379:VAL:O	2.43	0.51
1:A:142:MET:HG2	1:A:187:TYR:CE2	2.45	0.51
1:B:29:PRO:HB3	1:B:63:TYR:CZ	2.46	0.51
1:C:9:VAL:HG22	1:C:58:PHE:HB2	1.93	0.51
2:D:237:LEU:HB3	2:D:245:LEU:HD11	1.92	0.51
1:A:310:VAL:HA	1:A:327:CYS:O	2.10	0.50
1:C:360:ALA:HB2	1:C:371:THR:HG22	1.93	0.50
2:D:203:ALA:HA	2:D:208:LEU:HD11	1.93	0.50
1:C:353:GLY:O	1:C:356:SER:OG	2.24	0.50
1:A:50:LYS:HE2	1:A:127:GLN:H	1.76	0.50
2:D:53:ILE:HG21	2:D:60:MET:HE1	1.94	0.50
1:A:353:GLY:O	1:A:356:SER:OG	2.22	0.50
2:F:42:LYS:HG2	2:F:73:ILE:HD11	1.94	0.50
2:F:133:SER:HB2	2:F:209:TYR:CZ	2.46	0.50
2:E:42:LYS:HG2	2:E:73:ILE:HD11	1.93	0.50
2:D:102:GLY:HA2	2:D:181:PRO:HG2	1.94	0.49
2:E:139:VAL:HG21	2:E:145:TYR:HD2	1.76	0.49
1:A:269:ARG:HH21	1:A:291:ASP:H	1.60	0.49
2:E:345:LEU:HD22	2:E:361:MET:HB3	1.94	0.49
1:C:272:SER:O	1:C:275:ILE:HG12	2.12	0.49
2:F:125:HIS:ND1	2:F:209:TYR:OH	2.40	0.49
1:B:100:TYR:HD2	1:B:101:PHE:H	1.60	0.49
1:C:51:ILE:HD11	1:C:126:LEU:HB2	1.95	0.49
2:D:32:PRO:HD2	2:D:35:LEU:HD12	1.94	0.49
2:E:87:ALA:HB3	2:E:192:THR:HG23	1.95	0.49
1:A:251:ILE:HG22	1:A:256:LYS:HB3	1.95	0.49
2:E:22:PRO:HD2	2:E:25:LEU:HD12	1.94	0.49
1:B:373:LEU:HB3	1:B:377:VAL:HG11	1.94	0.49
2:D:56:GLN:CD	2:D:56:GLN:H	2.21	0.49
1:A:336:LYS:HD2	1:A:353:GLY:HA2	1.95	0.48
1:C:129:ILE:HG13	1:C:188:VAL:HG11	1.95	0.48
1:B:14:GLY:HA3	1:B:62:PHE:CE2	2.48	0.48
2:E:190:ARG:NH2	2:E:191:PRO:HD2	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:269:ARG:HH21	1:B:291:ASP:N	2.08	0.48
2:D:273:VAL:HA	2:D:290:CYS:O	2.13	0.48
1:A:19:THR:HA	1:A:22:ARG:HD3	1.94	0.48
1:A:29:PRO:HB3	1:A:63:TYR:CZ	2.49	0.48
1:C:14:GLY:HA3	1:C:62:PHE:CE2	2.48	0.48
1:C:310:VAL:HA	1:C:327:CYS:O	2.13	0.48
1:C:330:LEU:HD13	1:C:348:TRP:CE2	2.48	0.48
1:A:121:CYS:O	1:A:248:TRP:HA	2.14	0.48
1:A:106:MET:SD	1:A:110:PRO:HD2	2.54	0.48
2:E:44:VAL:HG23	2:E:46:VAL:HG23	1.96	0.48
1:C:106:MET:SD	1:C:110:PRO:HD2	2.54	0.48
1:B:192:ASP:OD1	1:B:195:ASN:ND2	2.40	0.48
2:E:18:THR:HA	2:E:21:PHE:O	2.14	0.47
2:F:44:VAL:HG23	2:F:46:VAL:HG23	1.95	0.47
1:C:373:LEU:HB3	1:C:377:VAL:HG11	1.96	0.47
2:F:136:VAL:HG11	2:F:171:LYS:HB3	1.95	0.47
1:C:155:PHE:HD2	1:C:182:ILE:HG22	1.79	0.47
1:B:292:VAL:HG13	1:B:310:VAL:HG13	1.96	0.47
1:C:251:ILE:HG22	1:C:256:LYS:HB3	1.96	0.47
2:F:145:TYR:HB2	2:F:172:ILE:HG21	1.95	0.47
1:A:60:ILE:HG22	1:A:86:LEU:HB2	1.96	0.47
1:A:102:ARG:NH1	1:A:198:GLU:OE2	2.47	0.47
1:A:155:PHE:HD2	1:A:182:ILE:HG22	1.79	0.47
1:B:268:PHE:HB3	1:B:275:ILE:HD11	1.97	0.47
2:E:145:TYR:CD2	2:E:172:ILE:HD13	2.50	0.47
2:E:203:ALA:HA	2:E:208:LEU:HD11	1.96	0.47
2:F:11:GLY:O	2:F:18:THR:OG1	2.29	0.47
1:A:322:VAL:HG12	1:A:339:ALA:H	1.80	0.46
1:A:353:GLY:N	1:A:379:VAL:O	2.44	0.46
1:A:360:ALA:HB2	1:A:371:THR:HG22	1.95	0.46
1:C:170:TYR:OH	1:C:226:ASP:HB2	2.15	0.46
1:B:306:ILE:HD12	1:B:324:LEU:HD12	1.96	0.46
1:C:294:ILE:HG12	1:C:312:ILE:HD12	1.97	0.46
1:C:312:ILE:HG22	1:C:316:VAL:HG11	1.96	0.46
1:B:43:HIS:HB2	1:B:44:PRO:HD3	1.98	0.46
2:D:94:ARG:NH2	2:D:184:LEU:O	2.48	0.46
2:D:151:GLU:OE2	2:D:154:THR:OG1	2.33	0.46
2:E:80:GLU:HG3	2:E:92:LEU:HD13	1.97	0.46
1:A:340:VAL:HB	1:A:357:ARG:HG3	1.96	0.46
1:B:122:CYS:HB3	1:B:248:TRP:HD1	1.80	0.46
1:B:272:SER:O	1:B:275:ILE:HG12	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:155:PHE:CD2	1:C:182:ILE:HG22	2.51	0.46
2:E:136:VAL:HG11	2:E:171:LYS:HB3	1.98	0.46
1:B:129:ILE:HG13	1:B:188:VAL:HG11	1.98	0.46
2:D:136:VAL:HG11	2:D:171:LYS:HB3	1.98	0.46
1:C:269:ARG:HA	1:C:269:ARG:HD3	1.70	0.46
1:C:117:ASN:ND2	1:C:119:ASP:OD1	2.49	0.46
1:C:166:GLU:HG3	1:C:237:LYS:HD2	1.98	0.46
2:D:145:TYR:CD2	2:D:172:ILE:HD13	2.51	0.46
2:F:186:LYS:HZ2	2:F:201:LYS:HD3	1.79	0.46
1:A:226:ASP:HB3	1:A:230:LEU:HD12	1.98	0.45
1:B:237:LYS:HB3	1:B:237:LYS:HE2	1.72	0.45
2:F:60:MET:HE3	2:F:64:LEU:HD11	1.98	0.45
1:B:5:LYS:O	1:B:111:SER:N	2.47	0.45
2:D:142:PRO:HB3	2:D:170:ASN:HA	1.99	0.45
1:A:342:ILE:O	1:A:359:GLN:HA	2.17	0.45
1:B:9:VAL:HG22	1:B:58:PHE:HB2	1.97	0.45
2:E:22:PRO:HD2	2:E:25:LEU:HB2	1.97	0.45
1:A:237:LYS:HE2	1:A:237:LYS:HB3	1.64	0.45
1:A:80:LYS:HB2	1:A:80:LYS:HE2	1.68	0.45
1:B:129:ILE:HD11	1:B:141:THR:HB	1.98	0.45
1:B:247:PHE:HB2	1:B:263:LEU:HD13	1.99	0.45
1:B:258:LEU:HD12	1:B:370:ILE:HD12	1.99	0.45
1:C:53:ASN:OD1	1:C:53:ASN:N	2.48	0.45
1:C:80:LYS:HE2	1:C:80:LYS:HB2	1.70	0.45
2:E:268:LEU:HB3	2:E:286:ARG:HD3	1.99	0.45
2:F:119:LYS:HE3	2:F:119:LYS:HB3	1.87	0.45
2:E:52:ALA:HB1	2:E:89:PRO:HB3	1.99	0.45
1:C:159:ILE:HD13	1:C:179:SER:HB2	1.98	0.45
1:A:269:ARG:HH21	1:A:291:ASP:N	2.15	0.44
1:B:71:TYR:CE2	1:B:75:ILE:HD11	2.51	0.44
1:B:172:GLU:HG2	1:B:227:GLN:HG3	1.99	0.44
1:B:332:ASP:O	1:B:349:LYS:HA	2.18	0.44
2:F:262:THR:HG23	2:F:280:ILE:HA	2.00	0.44
2:F:32:PRO:HD2	2:F:35:LEU:HD12	1.99	0.44
1:B:166:GLU:HG3	1:B:237:LYS:HD2	1.99	0.44
2:D:231:ARG:HD3	2:D:272:ASP:OD2	2.17	0.44
1:B:60:ILE:HG22	1:B:86:LEU:HB2	1.99	0.44
1:C:139:ILE:HA	1:C:190:THR:HG22	2.00	0.44
2:D:135:MET:SD	2:D:211:MET:HB3	2.58	0.44
1:A:312:ILE:HG23	1:A:316:VAL:HG11	1.99	0.44
2:D:22:PRO:HD2	2:D:25:LEU:HD12	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:136:VAL:CG1	2:F:171:LYS:HB3	2.48	0.44
2:F:273:VAL:HA	2:F:290:CYS:O	2.18	0.44
1:A:129:ILE:HD13	1:A:242:TYR:HB3	1.98	0.44
1:C:100:TYR:HD2	1:C:101:PHE:H	1.66	0.44
2:F:22:PRO:HB2	2:F:24:PRO:HD2	1.99	0.44
1:A:9:VAL:HG21	1:A:105:ILE:HD13	1.99	0.44
1:B:80:LYS:HB2	1:B:80:LYS:HE2	1.70	0.44
2:F:115:GLU:HB3	2:F:240:LYS:NZ	2.31	0.44
2:D:326:ILE:HB	2:D:343:VAL:HG13	2.00	0.43
2:F:157:VAL:HG22	2:F:208:LEU:HD13	1.99	0.43
1:C:342:ILE:O	1:C:359:GLN:HA	2.18	0.43
1:A:11:MET:HE1	1:A:97:ALA:HB3	1.99	0.43
1:A:272:SER:O	1:A:275:ILE:HG12	2.17	0.43
1:A:301:HIS:CG	1:A:320:PRO:HB3	2.54	0.43
1:A:109:LYS:N	1:A:110:PRO:HD3	2.34	0.43
1:A:155:PHE:CD2	1:A:182:ILE:HG22	2.53	0.43
1:C:170:TYR:HH	1:C:226:ASP:HB2	1.84	0.43
2:E:56:GLN:H	2:E:56:GLN:CD	2.27	0.43
2:F:48:GLU:HA	2:F:74:LYS:HB3	2.00	0.43
1:A:72:VAL:HG13	1:A:83:VAL:HB	2.01	0.43
1:C:71:TYR:CE2	1:C:75:ILE:HD11	2.54	0.43
2:D:11:GLY:O	2:D:18:THR:OG1	2.29	0.43
2:D:35:LEU:HD21	2:D:67:PHE:CD2	2.54	0.43
2:D:87:ALA:HB3	2:D:192:THR:HG23	2.00	0.43
2:D:136:VAL:CG1	2:D:171:LYS:HB3	2.48	0.43
2:D:28:PHE:N	2:D:31:LYS:O	2.50	0.43
2:D:161:VAL:HG12	2:D:164:PRO:HG3	2.01	0.43
2:F:29:ALA:O	2:F:30:ASN:HB2	2.19	0.43
1:B:312:ILE:HG22	1:B:316:VAL:HG11	2.00	0.43
2:E:32:PRO:HD2	2:E:35:LEU:HD12	2.01	0.43
2:F:30:ASN:OD1	2:F:258:ASP:HB2	2.18	0.43
2:F:87:ALA:HB3	2:F:192:THR:HG23	2.00	0.43
2:F:57:PRO:O	2:F:61:LEU:HG	2.18	0.43
2:F:282:GLU:OE1	2:F:300:LYS:HG3	2.19	0.43
1:B:19:THR:HA	1:B:22:ARG:HD3	2.00	0.43
2:D:173:ASN:HD21	2:D:177:TYR:HE1	1.67	0.43
2:E:95:ASP:OD1	2:E:95:ASP:N	2.50	0.43
1:B:8:ALA:HA	1:B:114:PHE:HB2	2.00	0.42
1:C:295:HIS:O	1:C:298:VAL:HG13	2.19	0.42
2:D:95:ASP:OD1	2:D:95:ASP:N	2.48	0.42
2:D:115:GLU:HB3	2:D:240:LYS:NZ	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:161:VAL:HG11	2:D:168:VAL:HG21	2.02	0.42
1:A:33:ILE:HA	1:A:34:PRO:HD3	1.93	0.42
1:A:119:ASP:OD1	1:A:119:ASP:N	2.52	0.42
1:C:156:GLY:HA2	1:C:175:GLU:HB3	2.00	0.42
1:A:166:GLU:HG3	1:A:237:LYS:HD2	2.01	0.42
1:C:50:LYS:HE2	1:C:127:GLN:N	2.28	0.42
1:A:306:ILE:HD12	1:A:324:LEU:HD12	2.01	0.42
1:B:99:TYR:HB2	1:B:197:ILE:HG21	2.02	0.42
1:B:322:VAL:HG12	1:B:339:ALA:H	1.85	0.42
2:E:53:ILE:HG21	2:E:60:MET:HE1	2.02	0.42
2:F:65:LYS:HE3	2:F:65:LYS:HB2	1.84	0.42
2:F:231:ARG:HD3	2:F:272:ASP:OD2	2.19	0.42
1:A:25:SER:HA	1:A:28:THR:O	2.18	0.42
1:C:295:HIS:CG	1:C:296:PRO:HD2	2.55	0.42
2:E:115:GLU:HB3	2:E:240:LYS:NZ	2.30	0.42
2:E:157:VAL:HG22	2:E:208:LEU:HD13	2.02	0.42
2:F:106:PHE:CE1	2:F:178:LEU:HD12	2.55	0.42
1:A:44:PRO:HG3	1:A:124:PHE:CZ	2.54	0.42
1:A:403:ASP:OD1	1:A:404:ILE:N	2.47	0.42
2:E:289:ARG:HD3	2:E:306:SER:HB3	2.01	0.42
1:B:307:GLY:CA	1:B:323:ARG:HH12	2.32	0.42
1:B:342:ILE:O	1:B:359:GLN:HA	2.19	0.42
1:C:236:LYS:H	1:C:236:LYS:HG2	1.59	0.42
1:C:311:SER:HB2	1:C:328:ILE:HG22	2.01	0.42
2:D:29:ALA:O	2:D:30:ASN:HB2	2.20	0.42
2:F:189:LEU:H	2:F:189:LEU:HG	1.71	0.42
1:B:361:SER:OG	1:B:369:GLY:HA2	2.20	0.42
1:C:43:HIS:HB2	1:C:44:PRO:HD3	2.02	0.42
2:F:257:VAL:HG21	2:F:263:ILE:HD11	2.00	0.42
1:C:159:ILE:HB	1:C:169:HIS:HB3	2.02	0.41
2:D:47:ASP:O	2:D:74:LYS:N	2.37	0.41
2:F:13:ARG:H	2:F:13:ARG:HG2	1.61	0.41
1:A:268:PHE:HB3	1:A:275:ILE:HD11	2.01	0.41
1:A:305:LYS:HG2	1:A:323:ARG:NH1	2.35	0.41
1:C:277:ALA:HB1	1:C:288:ILE:HD13	2.01	0.41
2:E:355:LEU:H	2:E:355:LEU:HG	1.49	0.41
1:B:29:PRO:O	1:B:33:ILE:HG13	2.21	0.41
1:B:236:LYS:H	1:B:236:LYS:HG2	1.52	0.41
1:A:307:GLY:N	1:A:324:LEU:O	2.52	0.41
1:B:41:ILE:C	1:B:44:PRO:HD2	2.45	0.41
1:C:173:LYS:HD2	1:C:173:LYS:HA	1.87	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:173:ASN:OD1	2:D:174:ALA:N	2.54	0.41
2:E:30:ASN:OD1	2:E:258:ASP:HB2	2.20	0.41
2:E:133:SER:HB2	2:E:209:TYR:OH	2.20	0.41
2:E:282:GLU:OE1	2:E:300:LYS:HG3	2.21	0.41
2:F:56:GLN:CD	2:F:56:GLN:H	2.27	0.41
2:F:95:ASP:OD1	2:F:95:ASP:N	2.50	0.41
2:F:289:ARG:HD3	2:F:306:SER:HB3	2.02	0.41
1:A:129:ILE:HD11	1:A:141:THR:HB	2.03	0.41
1:A:155:PHE:CZ	1:A:170:TYR:HE1	2.37	0.41
2:E:161:VAL:HG11	2:E:168:VAL:HG21	2.02	0.41
1:B:152:ALA:HB1	1:B:175:GLU:OE1	2.21	0.41
2:E:4:LEU:O	2:E:107:VAL:HA	2.19	0.41
1:A:47:ALA:HB1	1:A:50:LYS:NZ	2.36	0.41
1:A:100:TYR:HD2	1:A:101:PHE:H	1.68	0.41
1:B:51:ILE:HD11	1:B:126:LEU:HB2	2.03	0.41
1:B:310:VAL:HA	1:B:327:CYS:O	2.20	0.41
1:C:166:GLU:HG2	1:C:239:LEU:O	2.19	0.41
2:F:345:LEU:HD22	2:F:361:MET:HB3	2.02	0.41
1:A:168:LEU:O	1:A:234:ALA:HB1	2.20	0.41
1:B:301:HIS:CG	1:B:320:PRO:HB3	2.56	0.41
2:D:139:VAL:HG21	2:D:145:TYR:HD2	1.85	0.41
2:E:29:ALA:O	2:E:30:ASN:HB2	2.20	0.41
2:F:28:PHE:N	2:F:31:LYS:O	2.51	0.41
1:A:17:LYS:C	1:A:19:THR:H	2.29	0.41
1:C:247:PHE:HB2	1:C:263:LEU:HD13	2.03	0.41
1:A:375:GLU:O	1:A:393:ASN:N	2.38	0.41
1:C:51:ILE:HD11	1:C:126:LEU:CB	2.51	0.41
2:E:282:GLU:CD	2:E:299:LYS:HA	2.46	0.41
1:A:53:ASN:OD1	1:A:53:ASN:N	2.50	0.40
1:A:175:GLU:HG3	1:A:176:THR:H	1.86	0.40
1:B:109:LYS:N	1:B:110:PRO:HD3	2.36	0.40
1:B:34:PRO:HA	1:B:39:PRO:HA	2.03	0.40
1:C:355:TRP:CE2	2:F:286:ARG:HB2	2.57	0.40
2:D:27:ASP:HA	2:D:32:PRO:HA	2.02	0.40
2:E:65:LYS:HB2	2:E:65:LYS:HE3	1.81	0.40
1:A:129:ILE:HG13	1:A:188:VAL:HG11	2.03	0.40
1:C:176:THR:O	1:C:177:PHE:HB3	2.21	0.40
2:D:296:VAL:HG23	2:D:313:SER:C	2.46	0.40
1:B:239:LEU:HD22	1:B:239:LEU:HA	1.90	0.40
1:C:306:ILE:HD12	1:C:324:LEU:HD12	2.02	0.40
2:D:48:GLU:HA	2:D:74:LYS:HB3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:173:LYS:HA	1:A:173:LYS:HD2	1.91	0.40
1:B:176:THR:O	1:B:177:PHE:HB3	2.22	0.40
1:C:175:GLU:HG3	1:C:176:THR:H	1.87	0.40
2:D:187:ILE:H	2:D:187:ILE:HG13	1.61	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	383/406 (94%)	346 (90%)	35 (9%)	2 (0%)	24	58
1	B	383/406 (94%)	345 (90%)	36 (9%)	2 (0%)	24	58
1	C	371/406 (91%)	335 (90%)	34 (9%)	2 (0%)	24	58
2	D	359/361 (99%)	341 (95%)	18 (5%)	0	100	100
2	E	355/361 (98%)	336 (95%)	19 (5%)	0	100	100
2	F	349/361 (97%)	333 (95%)	16 (5%)	0	100	100
All	All	2200/2301 (96%)	2036 (92%)	158 (7%)	6 (0%)	36	66

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	177	PHE
1	B	177	PHE
1	C	177	PHE
1	A	173	LYS
1	B	173	LYS
1	C	173	LYS

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	329/355 (93%)	305 (93%)	24 (7%)	13	39
1	B	329/355 (93%)	305 (93%)	24 (7%)	13	39
1	C	316/355 (89%)	293 (93%)	23 (7%)	13	39
2	D	308/310 (99%)	289 (94%)	19 (6%)	16	44
2	E	304/310 (98%)	287 (94%)	17 (6%)	19	46
2	F	302/310 (97%)	286 (95%)	16 (5%)	20	47
All	All	1888/1995 (95%)	1765 (94%)	123 (6%)	15	42

All (123) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	ARG
1	A	30	LYS
1	A	81	ILE
1	A	98	LEU
1	A	113	VAL
1	A	141	THR
1	A	172	GLU
1	A	173	LYS
1	A	176	THR
1	A	180	ASP
1	A	186	VAL
1	A	188	VAL
1	A	201	TYR
1	A	227	GLN
1	A	233	LEU
1	A	236	LYS
1	A	239	LEU
1	A	250	GLN
1	A	252	LYS
1	A	253	THR
1	A	269	ARG
1	A	287	THR

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Mol	Chain	Res	Type
1	A	310	VAL
1	A	361	SER
1	B	20	ARG
1	B	30	LYS
1	B	81	ILE
1	B	98	LEU
1	B	113	VAL
1	B	141	THR
1	B	172	GLU
1	B	173	LYS
1	B	176	THR
1	B	179	SER
1	B	180	ASP
1	B	186	VAL
1	B	188	VAL
1	B	201	TYR
1	B	227	GLN
1	B	233	LEU
1	B	236	LYS
1	B	239	LEU
1	B	250	GLN
1	B	252	LYS
1	B	253	THR
1	B	269	ARG
1	B	287	THR
1	B	310	VAL
1	C	20	ARG
1	C	30	LYS
1	C	81	ILE
1	C	98	LEU
1	C	113	VAL
1	C	141	THR
1	C	172	GLU
1	C	173	LYS
1	C	176	THR
1	C	180	ASP
1	C	188	VAL
1	C	201	TYR
1	C	227	GLN
1	C	233	LEU
1	C	236	LYS
1	C	239	LEU

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Mol	Chain	Res	Type
1	C	250	GLN
1	C	252	LYS
1	C	253	THR
1	C	269	ARG
1	C	287	THR
1	C	310	VAL
1	C	361	SER
2	D	42	LYS
2	D	47	ASP
2	D	69	THR
2	D	82	GLU
2	D	84	LEU
2	D	86	THR
2	D	128	HIS
2	D	157	VAL
2	D	166	LEU
2	D	170	ASN
2	D	176	ILE
2	D	187	ILE
2	D	189	LEU
2	D	192	THR
2	D	208	LEU
2	D	238	ARG
2	D	257	VAL
2	D	296	VAL
2	D	355	LEU
2	E	42	LYS
2	E	47	ASP
2	E	69	THR
2	E	86	THR
2	E	128	HIS
2	E	157	VAL
2	E	166	LEU
2	E	170	ASN
2	E	176	ILE
2	E	187	ILE
2	E	189	LEU
2	E	192	THR
2	E	208	LEU
2	E	238	ARG
2	E	257	VAL
2	E	296	VAL

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Mol	Chain	Res	Type
2	E	355	LEU
2	F	42	LYS
2	F	47	ASP
2	F	69	THR
2	F	86	THR
2	F	128	HIS
2	F	157	VAL
2	F	166	LEU
2	F	170	ASN
2	F	187	ILE
2	F	189	LEU
2	F	192	THR
2	F	208	LEU
2	F	238	ARG
2	F	257	VAL
2	F	296	VAL
2	F	355	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	27	ASN
1	A	112	HIS
1	B	112	HIS
1	C	112	HIS
1	C	309	ASN
2	D	37	GLN
2	E	37	GLN
2	E	54	ASN
2	F	54	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](#)

12 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	$\# Z > 2$
3	SO4	B	501	-	4,4,4	0.24	0	6,6,6	0.06	0
3	SO4	A	502	-	4,4,4	0.24	0	6,6,6	0.08	0
3	SO4	E	402	-	4,4,4	0.24	0	6,6,6	0.10	0
3	SO4	F	402	-	4,4,4	0.24	0	6,6,6	0.06	0
3	SO4	D	404	-	4,4,4	0.24	0	6,6,6	0.09	0
3	SO4	F	401	-	4,4,4	0.24	0	6,6,6	0.11	0
3	SO4	A	503	-	4,4,4	0.23	0	6,6,6	0.05	0
3	SO4	D	402	-	4,4,4	0.24	0	6,6,6	0.10	0
3	SO4	D	403	-	4,4,4	0.23	0	6,6,6	0.09	0
3	SO4	A	501	-	4,4,4	0.24	0	6,6,6	0.07	0
3	SO4	D	401	-	4,4,4	0.24	0	6,6,6	0.07	0
3	SO4	E	401	-	4,4,4	0.23	0	6,6,6	0.06	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 ⓘ

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	A	387/406 (95%)	-0.43	0	100	100	18, 102, 153, 238	1 (0%)
1	B	387/406 (95%)	-0.41	0	100	100	63, 96, 167, 276	0
1	C	381/406 (93%)	0.03	4 (1%)	79	53	7, 178, 247, 322	8 (2%)
2	D	361/361 (100%)	-0.13	1 (0%)	90	74	40, 129, 198, 279	1 (0%)
2	E	359/361 (99%)	-0.24	2 (0%)	85	63	46, 146, 235, 368	2 (0%)
2	F	355/361 (98%)	-0.05	1 (0%)	90	74	8, 152, 216, 322	4 (1%)
All	All	2230/2301 (96%)	-0.21	8 (0%)	88	69	7, 128, 221, 368	16 (0%)

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	195	GLU	3.6
2	D	207	GLY	2.8
1	C	225	LEU	2.4
1	C	235	GLY	2.3
2	F	157	VAL	2.2
1	C	384	ALA	2.2
2	E	212	VAL	2.1
1	C	98	LEU	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
3	SO4	F	402	5/5	0.95	0.14	153,158,162,165	0
3	SO4	D	403	5/5	0.96	0.13	141,142,150,152	0
3	SO4	A	501	5/5	0.96	0.09	192,192,195,196	0
3	SO4	E	402	5/5	0.97	0.10	148,149,152,153	0
3	SO4	F	401	5/5	0.97	0.09	151,159,163,170	0
3	SO4	A	502	5/5	0.97	0.09	152,153,158,164	0
3	SO4	A	503	5/5	0.98	0.09	129,130,136,145	0
3	SO4	E	401	5/5	0.98	0.05	124,128,133,135	0
3	SO4	B	501	5/5	0.98	0.13	77,78,83,88	5
3	SO4	D	401	5/5	0.98	0.08	146,147,156,158	0
3	SO4	D	402	5/5	0.98	0.12	131,134,139,141	0
3	SO4	D	404	5/5	0.99	0.06	137,139,148,151	0

6.5 Other polymers [i](#)

There are no such residues in this entry.