



Full wwPDB X-ray Structure Validation Report ⓘ

May 3, 2025 – 08:46 AM EDT

PDB ID : 3MV9 / pdb_00003mv9
Title : Crystal Structure of the TK3-Gln55Ala TCR in complex with HLA-B*3501/HPVG
Authors : Gras, S.; Chen, Z.; Miles, J.J.; Liu, Y.C.; Bell, M.J.; Sullivan, L.C.; Kjer-Nielsen, L.; Brennan, R.M.; Burrows, J.M.; Neller, M.A.; Khanna, R.; Purcell, A.W.; Brooks, A.G.; McCluskey, J.; Rossjohn, J.; Burrows, S.R.
Deposited on : 2010-05-03
Resolution : 2.70 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 Phenix2.0rc1
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.006 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

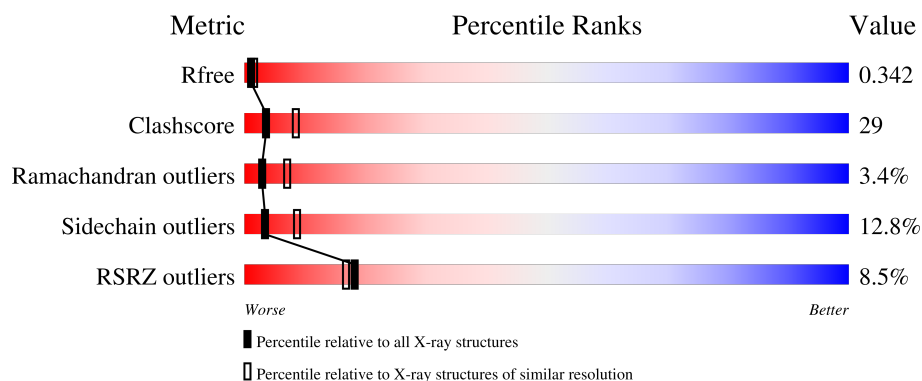
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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}	164625	3333 (2.70-2.70)
Clashscore	180529	3684 (2.70-2.70)
Ramachandran outliers	177936	3633 (2.70-2.70)
Sidechain outliers	177891	3633 (2.70-2.70)
RSRZ outliers	164620	3333 (2.70-2.70)

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	276	
2	B	100	
3	C	11	
4	D	200	

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Mol	Chain	Length	Quality of chain
5	E	241	<div><div><div>%</div><div><div></div><div>55%</div><div>34%</div><div>10%</div><div></div></div><div></div></div></div>

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 6745 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 HLA class I histocompatibility antigen, B-35 alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	276	Total	C	N	O	S	0	0	0
			2254	1405	411	431	7			

- Molecule 2 is a protein called Beta-2-microglobulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	100	Total	C	N	O	S	0	0	0
			837	533	141	159	4			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	0	MET	-	initiating methionine	UNP P61769

- Molecule 3 is a protein called HPVG peptide from Epstein-Barr nuclear antigen 1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	11	Total	C	N	O	0	0	0
			95	62	13	20			

- Molecule 4 is a protein called alpha chain of the TK3 TCR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	200	Total	C	N	O	S	0	1	0
			1568	977	261	323	7			

- Molecule 5 is a protein called beta chain of the TK3 TCR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	241	Total	C	N	O	S	0	2	0
			1924	1210	335	374	5			

- Molecule 6 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	D	1	Total	O	S	0	0
			5	4	1		

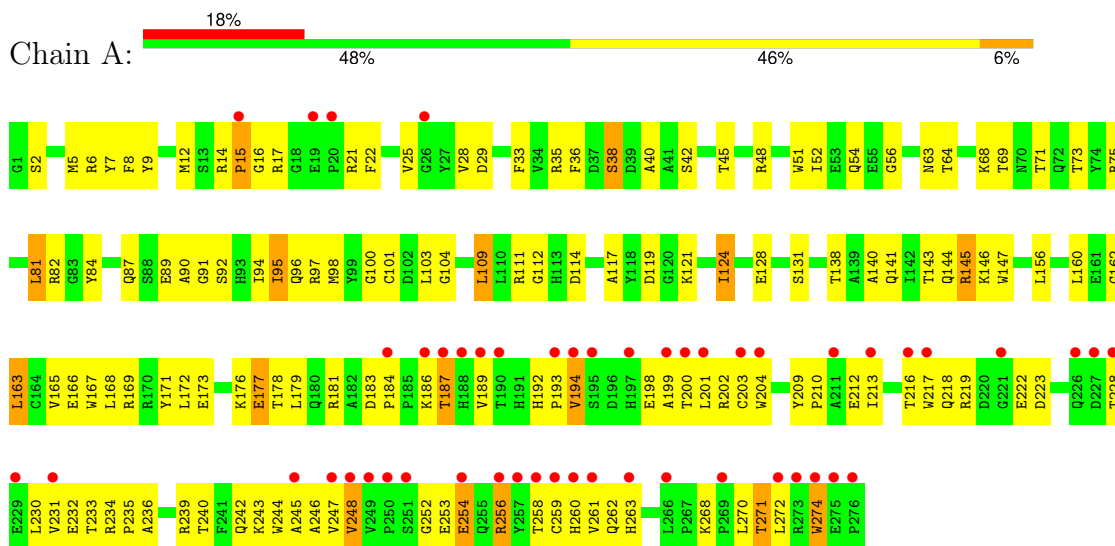
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	14	Total	O	0	0
			14	14		
7	B	4	Total	O	0	0
			4	4		
7	C	4	Total	O	0	0
			4	4		
7	D	18	Total	O	0	0
			18	18		
7	E	22	Total	O	0	0
			22	22		

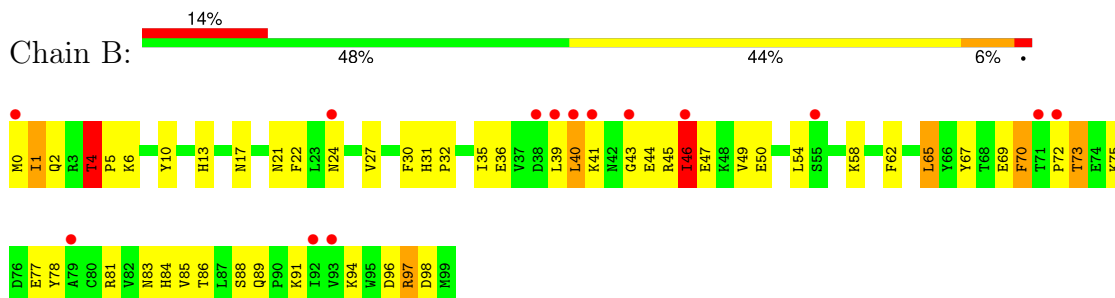
3 Residue-property plots

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: HLA class I histocompatibility antigen, B-35 alpha chain



- Molecule 2: Beta-2-microglobulin

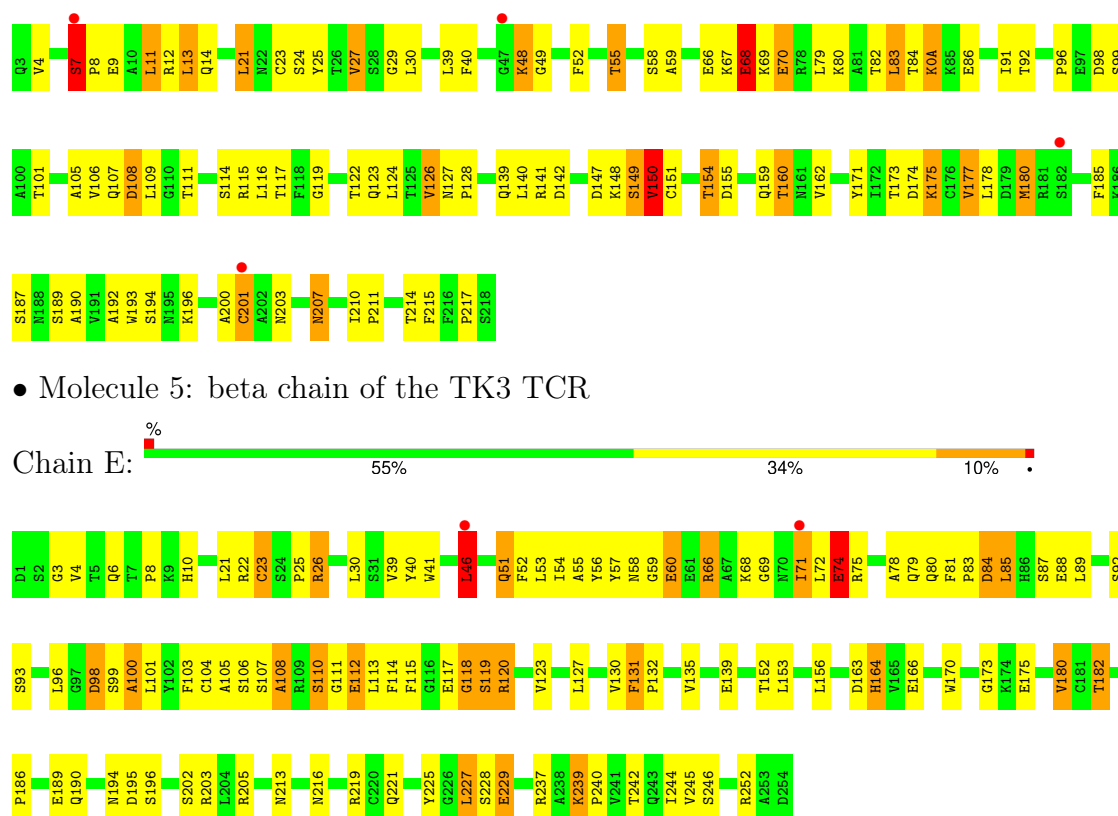


- Molecule 3: HPVG peptide from Epstein-Barr nuclear antigen 1



- Molecule 4: alpha chain of the TK3 TCR





• Molecule 5: beta chain of the TK3 TCR

4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	44.90Å 62.57Å 98.14Å 92.04° 102.29° 109.18°	Depositor
Resolution (Å)	39.25 – 2.70 39.25 – 2.70	Depositor EDS
% Data completeness (in resolution range)	83.7 (39.25-2.70) 94.5 (39.25-2.70)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.79 (at 2.69Å)	Xtriage
Refinement program	REFMAC, PHENIX 1.4_4	Depositor
R, R_{free}	0.234 , 0.331 0.250 , 0.342	Depositor DCC
R_{free} test set	1285 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	45.4	Xtriage
Anisotropy	0.625	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 44.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.019 for h,-h-k,-h-l	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	6745	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.76% 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: 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	0.45	0/2317	0.84	3/3150 (0.1%)
2	B	0.37	0/860	0.85	2/1162 (0.2%)
3	C	0.48	0/99	0.96	0/133
4	D	0.52	0/1601	1.01	5/2167 (0.2%)
5	E	0.49	0/1973	0.95	5/2682 (0.2%)
All	All	0.47	0/6850	0.92	15/9294 (0.2%)

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	7	SER	CA-C-N	-8.08	109.74	119.84
4	D	7	SER	C-N-CA	-8.08	109.74	119.84
5	E	239	LYS	CA-C-N	7.63	129.38	119.84
5	E	239	LYS	C-N-CA	7.63	129.38	119.84
5	E	131	PHE	CA-C-N	7.41	125.00	119.66
5	E	131	PHE	C-N-CA	7.41	125.00	119.66
1	A	194	VAL	N-CA-C	6.51	113.17	106.21
1	A	56	GLY	CA-C-N	6.04	125.52	119.24
1	A	56	GLY	C-N-CA	6.04	125.52	119.24
4	D	49	GLY	CA-C-N	5.95	126.30	119.93
4	D	49	GLY	C-N-CA	5.95	126.30	119.93
5	E	98	ASP	N-CA-C	-5.49	106.26	113.12
4	D	196	LYS	CB-CA-C	-5.43	110.29	116.54
2	B	4	THR	CA-C-N	5.24	125.16	119.76
2	B	4	THR	C-N-CA	5.24	125.16	119.76

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	2254	0	2117	134	0
2	B	837	0	803	48	0
3	C	95	0	76	8	0
4	D	1568	0	1491	91	0
5	E	1924	0	1825	106	0
6	D	5	0	0	0	0
7	A	14	0	0	1	0
7	B	4	0	0	0	0
7	C	4	0	0	1	0
7	D	18	0	0	2	0
7	E	22	0	0	2	0
All	All	6745	0	6312	375	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 29.

All (375) 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)
4:D:68:GLU:HB3	4:D:69:LYS:HA	1.25	1.17
4:D:0(A):LYS:H	4:D:0(A):LYS:HD2	1.23	0.99
5:E:59:GLY:CA	5:E:60:GLU:HB2	1.93	0.98
1:A:103:LEU:HD13	1:A:168:LEU:HD23	1.41	0.98
2:B:35:ILE:HG23	2:B:36:GLU:H	1.28	0.97
4:D:68:GLU:HB3	4:D:69:LYS:CA	1.96	0.96
5:E:135:VAL:HG22	5:E:245:VAL:HG12	1.52	0.92
5:E:59:GLY:HA3	5:E:60:GLU:HB2	1.49	0.92
4:D:142:ASP:HB3	4:D:147:ASP:HA	1.51	0.89
4:D:14:GLN:NE2	4:D:127:ASN:HD22	1.70	0.89
5:E:8:PRO:O	5:E:119:SER:HB2	1.74	0.88
1:A:145:ARG:HG3	1:A:145:ARG:HH11	1.38	0.86
5:E:3:GLY:HA3	5:E:26:ARG:HG2	1.56	0.86
5:E:110:SER:N	5:E:111:GLY:HA2	1.90	0.84
5:E:22:ARG:HG2	5:E:23:CYS:H	1.40	0.83
2:B:40:LEU:H	2:B:40:LEU:HD23	1.42	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:15:PRO:HG3	1:A:92:SER:HB2	1.61	0.83
4:D:0(A):LYS:H	4:D:0(A):LYS:CD	1.91	0.83
4:D:8:PRO:O	4:D:122:THR:HG23	1.79	0.82
5:E:68:LYS:HE3	5:E:71:ILE:HD11	1.59	0.82
1:A:145:ARG:HH11	1:A:145:ARG:CG	1.93	0.82
5:E:84:ASP:O	5:E:85:LEU:HG	1.79	0.81
5:E:110:SER:H	5:E:111:GLY:HA2	1.43	0.81
1:A:200:THR:HA	1:A:248:VAL:HG13	1.62	0.81
2:B:46:ILE:HG23	2:B:46:ILE:O	1.79	0.80
5:E:75:ARG:HD3	5:E:93:SER:HB2	1.63	0.80
4:D:7:SER:HB3	4:D:8:PRO:HD3	1.64	0.80
5:E:59:GLY:N	5:E:60:GLU:HB2	1.97	0.79
4:D:14:GLN:HE22	4:D:127:ASN:HD22	1.27	0.78
4:D:174:ASP:O	4:D:175:LYS:HB3	1.82	0.78
1:A:111:ARG:HH21	1:A:128:GLU:HB2	1.46	0.78
4:D:150:VAL:HG23	4:D:193:TRP:HB3	1.67	0.76
4:D:0(A):LYS:HD2	4:D:0(A):LYS:N	2.00	0.76
2:B:35:ILE:HG23	2:B:36:GLU:N	2.00	0.76
1:A:219:ARG:H	1:A:222:GLU:HB2	1.51	0.75
1:A:202:ARG:HD3	1:A:246:ALA:HB2	1.68	0.74
1:A:234:ARG:HE	1:A:242:GLN:HE21	1.33	0.74
4:D:14:GLN:HE22	4:D:127:ASN:ND2	1.85	0.74
5:E:22:ARG:HG2	5:E:23:CYS:N	2.02	0.73
4:D:21:LEU:N	4:D:21:LEU:HD12	2.03	0.73
5:E:21:LEU:HD12	5:E:89:LEU:HD23	1.72	0.72
3:C:8:TYR:CZ	5:E:108:ALA:HB2	2.25	0.72
5:E:74:GLU:HG2	5:E:75:ARG:N	2.04	0.71
1:A:234:ARG:HG3	2:B:10:TYR:CZ	2.26	0.71
4:D:40:PHE:CE1	4:D:55:THR:HB	2.25	0.70
1:A:14:ARG:NH2	1:A:21:ARG:HB2	2.06	0.70
4:D:79:LEU:HD12	4:D:79:LEU:N	2.07	0.70
5:E:194:ASN:C	5:E:196:SER:H	2.00	0.70
1:A:259:CYS:HB3	1:A:272:LEU:HD11	1.74	0.69
4:D:96:PRO:HA	4:D:126:VAL:HB	1.74	0.69
5:E:59:GLY:H	5:E:60:GLU:HB2	1.54	0.69
5:E:110:SER:N	5:E:111:GLY:CA	2.55	0.69
1:A:189:VAL:HA	1:A:202:ARG:O	1.92	0.69
1:A:69:THR:O	1:A:73:THR:HG23	1.92	0.68
2:B:4:THR:HA	2:B:86:THR:HG21	1.75	0.68
2:B:84:HIS:ND1	2:B:86:THR:HG22	2.08	0.68
5:E:180:VAL:HA	5:E:203:ARG:O	1.93	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:175:LYS:HA	4:D:189:SER:O	1.95	0.67
5:E:237:ARG:HH12	5:E:240:PRO:HG3	1.59	0.67
4:D:23:CYS:O	4:D:86:GLU:HB2	1.95	0.67
2:B:24:ASN:ND2	2:B:67:TYR:HB3	2.09	0.67
1:A:51:TRP:HZ3	1:A:52:ILE:HD13	1.59	0.66
4:D:48:LYS:H	4:D:48:LYS:HD2	1.61	0.66
5:E:81:PHE:HB3	5:E:83:PRO:HD2	1.78	0.66
4:D:105:ALA:HB1	4:D:116:LEU:HD22	1.76	0.66
4:D:69:LYS:O	4:D:70:GLU:HB2	1.95	0.66
5:E:59:GLY:CA	5:E:60:GLU:CB	2.73	0.65
5:E:107:SER:O	5:E:108:ALA:CB	2.44	0.65
1:A:89:GLU:O	1:A:91:GLY:HA3	1.97	0.65
1:A:6:ARG:HG2	1:A:6:ARG:HH11	1.60	0.64
1:A:203:CYS:SG	1:A:272:LEU:HD21	2.37	0.64
2:B:35:ILE:CG2	2:B:36:GLU:H	2.08	0.64
1:A:14:ARG:HH21	1:A:21:ARG:HB2	1.63	0.63
1:A:202:ARG:HH12	2:B:98:ASP:HB3	1.63	0.63
5:E:68:LYS:HG3	5:E:71:ILE:HD11	1.80	0.63
1:A:112:GLY:HA3	1:A:160:LEU:HD13	1.81	0.63
2:B:45:ARG:HH11	2:B:47:GLU:HB2	1.64	0.63
2:B:45:ARG:O	2:B:46:ILE:HB	1.99	0.63
3:C:8:TYR:OH	5:E:108:ALA:HB2	2.00	0.62
1:A:2:SER:HB3	1:A:104:GLY:O	2.00	0.62
4:D:174:ASP:O	4:D:175:LYS:CB	2.47	0.62
5:E:41:TRP:O	5:E:53:LEU:HB2	2.00	0.62
3:C:7:ASP:HB3	3:C:8:TYR:CD1	2.35	0.61
4:D:201:CYS:C	4:D:203:ASN:H	2.08	0.61
1:A:199:ALA:HA	7:A:277:HOH:O	2.00	0.61
4:D:180:MET:HE2	5:E:205:ARG:HD3	1.83	0.61
4:D:207:ASN:H	4:D:207:ASN:ND2	1.97	0.61
4:D:27:VAL:HG22	4:D:108:ASP:CG	2.24	0.61
4:D:200:ALA:O	4:D:201:CYS:HB2	2.00	0.61
1:A:6:ARG:HG2	1:A:6:ARG:NH1	2.16	0.61
1:A:94:ILE:HG22	1:A:119:ASP:HA	1.82	0.61
1:A:202:ARG:NH1	2:B:98:ASP:HB3	2.15	0.61
2:B:44:GLU:HG3	2:B:81:ARG:NH1	2.16	0.61
1:A:219:ARG:H	1:A:222:GLU:CB	2.13	0.60
1:A:95:ILE:HG13	1:A:95:ILE:O	2.01	0.60
2:B:2:GLN:HG2	2:B:32:PRO:HD3	1.84	0.60
4:D:48:LYS:HD2	4:D:48:LYS:N	2.16	0.60
5:E:72:LEU:O	5:E:75:ARG:N	2.35	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:173:GLU:O	1:A:176:LYS:HG2	2.02	0.60
4:D:0(A):LYS:CD	4:D:0(A):LYS:N	2.63	0.60
5:E:57:TYR:CD2	5:E:58:ASN:N	2.70	0.59
1:A:15:PRO:HA	1:A:91:GLY:C	2.28	0.59
4:D:13:LEU:HD22	4:D:124:LEU:CD1	2.33	0.59
5:E:78:ALA:HB2	5:E:89:LEU:HA	1.85	0.59
2:B:41:LYS:C	2:B:43:GLY:H	2.11	0.58
2:B:70:PHE:HD1	2:B:78:TYR:CZ	2.20	0.58
5:E:135:VAL:CG2	5:E:245:VAL:HG12	2.30	0.58
1:A:14:ARG:HB3	1:A:17:ARG:HE	1.67	0.58
2:B:46:ILE:O	2:B:46:ILE:CG2	2.49	0.58
1:A:103:LEU:HD11	1:A:165:VAL:HG13	1.84	0.58
5:E:25:PRO:HB3	5:E:106:SER:HB2	1.85	0.58
5:E:68:LYS:HE3	5:E:71:ILE:CD1	2.31	0.58
1:A:209:TYR:CG	1:A:210:PRO:HA	2.39	0.57
5:E:78:ALA:HB2	5:E:89:LEU:HD12	1.87	0.57
1:A:145:ARG:CG	1:A:145:ARG:NH1	2.60	0.57
4:D:117:THR:HA	7:D:233:HOH:O	2.05	0.57
4:D:154:THR:OG1	4:D:155:ASP:N	2.38	0.57
1:A:15:PRO:C	1:A:17:ARG:H	2.12	0.57
5:E:66[A]:ARG:O	5:E:66[A]:ARG:HG3	2.05	0.57
2:B:22:PHE:CE1	2:B:69:GLU:HG2	2.39	0.56
4:D:40:PHE:HD1	4:D:52:PHE:HE2	1.52	0.56
4:D:178:LEU:HD12	4:D:178:LEU:H	1.70	0.56
4:D:52:PHE:HZ	4:D:55:THR:HG22	1.69	0.56
5:E:39:VAL:HG11	5:E:87:SER:CB	2.35	0.56
1:A:201:LEU:HB2	1:A:247:VAL:HG23	1.88	0.56
5:E:59:GLY:H	5:E:60:GLU:CB	2.18	0.56
4:D:215:PHE:CD2	4:D:217:PRO:HD3	2.40	0.56
5:E:26:ARG:NH1	5:E:114:PHE:CE2	2.74	0.56
1:A:218:GLN:CG	1:A:222:GLU:H	2.19	0.56
4:D:29:GLY:O	4:D:108:ASP:HA	2.05	0.55
4:D:123:GLN:C	4:D:123:GLN:OE1	2.49	0.55
5:E:163:ASP:OD1	5:E:186:PRO:HG2	2.06	0.55
1:A:218:GLN:HG2	1:A:222:GLU:H	1.71	0.55
4:D:24:SER:HA	4:D:86:GLU:HB3	1.89	0.55
5:E:57:TYR:CD2	5:E:58:ASN:HB2	2.42	0.55
1:A:218:GLN:HB2	1:A:258:THR:HG23	1.88	0.55
5:E:79:GLN:HG2	5:E:80:GLN:N	2.22	0.55
5:E:98:ASP:O	5:E:99:SER:C	2.50	0.55
4:D:21:LEU:N	4:D:21:LEU:CD1	2.68	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:84:HIS:CE1	2:B:85:VAL:HG12	2.41	0.55
5:E:59:GLY:N	5:E:60:GLU:CB	2.69	0.55
5:E:68:LYS:CE	5:E:71:ILE:HD11	2.32	0.55
5:E:40:TYR:CE2	5:E:107:SER:HB3	2.43	0.54
2:B:40:LEU:H	2:B:40:LEU:CD2	2.18	0.54
5:E:72:LEU:O	5:E:74:GLU:C	2.50	0.54
7:C:61:HOH:O	5:E:66[A]:ARG:HD3	2.08	0.54
2:B:13:HIS:H	2:B:21:ASN:HD21	1.55	0.54
1:A:15:PRO:HD2	1:A:17:ARG:CZ	2.38	0.54
1:A:35:ARG:HD3	1:A:48:ARG:HH21	1.73	0.54
1:A:94:ILE:CG2	1:A:119:ASP:HA	2.37	0.54
1:A:9:TYR:O	1:A:96:GLN:HA	2.07	0.54
2:B:89:GLN:HG3	2:B:91:LYS:NZ	2.22	0.54
4:D:162:VAL:HG21	4:D:190:ALA:HB2	1.89	0.54
5:E:46:LEU:HG	5:E:120:ARG:NH2	2.23	0.54
4:D:79:LEU:HD12	4:D:79:LEU:H	1.73	0.53
4:D:180:MET:CE	5:E:205:ARG:HD3	2.37	0.53
2:B:72:PRO:O	2:B:73:THR:HG23	2.07	0.53
1:A:176:LYS:O	1:A:177:GLU:CB	2.56	0.53
1:A:192:HIS:HE1	2:B:98:ASP:CG	2.16	0.53
1:A:189:VAL:HG13	1:A:274:TRP:HB3	1.91	0.53
1:A:198:GLU:HG2	1:A:252:GLY:HA3	1.91	0.53
2:B:5:PRO:HA	2:B:30:PHE:HB3	1.90	0.53
5:E:219:ARG:NH2	7:E:37:HOH:O	2.42	0.53
1:A:259:CYS:HB3	1:A:272:LEU:CD1	2.37	0.53
5:E:112:GLU:H	5:E:112:GLU:CD	2.17	0.53
1:A:89:GLU:C	1:A:91:GLY:HA3	2.34	0.52
4:D:7:SER:HB3	4:D:8:PRO:CD	2.38	0.52
5:E:21:LEU:HD22	5:E:119:SER:OG	2.10	0.52
2:B:24:ASN:HD22	2:B:67:TYR:HB3	1.74	0.52
4:D:128:PRO:CG	4:D:177:VAL:HG21	2.38	0.52
4:D:178:LEU:CD2	5:E:205:ARG:HB2	2.39	0.52
2:B:54:LEU:HD11	2:B:62:PHE:CD1	2.45	0.52
5:E:139:GLU:OE2	5:E:252:ARG:HD3	2.10	0.52
1:A:259:CYS:HB3	1:A:272:LEU:CG	2.40	0.52
5:E:99:SER:O	5:E:100:ALA:HB2	2.09	0.52
1:A:169:ARG:HA	1:A:172:LEU:HD12	1.90	0.51
3:C:6:ALA:HB3	3:C:9:PHE:CE1	2.44	0.51
1:A:8:PHE:HB2	1:A:25:VAL:CG2	2.41	0.51
1:A:124:ILE:HD11	1:A:144:GLN:HB2	1.92	0.51
1:A:200:THR:HG22	1:A:202:ARG:HH21	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:44:GLU:HG3	2:B:81:ARG:CZ	2.40	0.51
4:D:140:LEU:O	4:D:149:SER:HA	2.10	0.51
4:D:142:ASP:HB2	4:D:148:LYS:H	1.73	0.51
5:E:74:GLU:HG2	5:E:75:ARG:H	1.73	0.51
4:D:207:ASN:H	4:D:207:ASN:HD22	1.57	0.51
1:A:203:CYS:HB2	1:A:217:TRP:CZ2	2.46	0.51
1:A:163:LEU:CD2	1:A:167:TRP:HE1	2.24	0.51
1:A:176:LYS:O	1:A:177:GLU:HB3	2.09	0.51
4:D:201:CYS:C	4:D:203:ASN:N	2.68	0.51
5:E:72:LEU:C	5:E:75:ARG:N	2.67	0.51
4:D:68:GLU:CB	4:D:69:LYS:CA	2.80	0.51
1:A:230:LEU:HD13	1:A:245:ALA:HB2	1.91	0.51
4:D:21:LEU:CD1	4:D:21:LEU:H	2.24	0.51
2:B:17:ASN:HD22	2:B:73:THR:HA	1.75	0.50
1:A:14:ARG:HB2	1:A:17:ARG:HG3	1.94	0.50
1:A:15:PRO:HA	1:A:91:GLY:O	2.10	0.50
4:D:21:LEU:HD12	4:D:21:LEU:H	1.74	0.50
1:A:22:PHE:H	1:A:38:SER:CB	2.25	0.50
1:A:231:VAL:HG21	1:A:244:TRP:CZ2	2.47	0.50
1:A:15:PRO:HD2	1:A:17:ARG:NH2	2.26	0.50
4:D:128:PRO:HG3	4:D:177:VAL:HG21	1.94	0.50
2:B:96:ASP:OD1	2:B:97:ARG:N	2.44	0.49
1:A:177:GLU:O	1:A:181:ARG:HB2	2.11	0.49
2:B:39:LEU:HB2	2:B:46:ILE:HG21	1.93	0.49
4:D:160:THR:HG21	4:D:211:PRO:HD3	1.94	0.49
1:A:222:GLU:HG3	1:A:223:ASP:H	1.78	0.49
1:A:260:HIS:CE1	1:A:271:THR:HG23	2.48	0.49
4:D:171:TYR:O	4:D:192:ALA:HA	2.12	0.49
5:E:84:ASP:OD1	5:E:85:LEU:N	2.45	0.49
1:A:15:PRO:C	1:A:17:ARG:N	2.70	0.49
5:E:39:VAL:HG11	5:E:87:SER:HB2	1.93	0.49
5:E:54:ILE:HD13	5:E:56:TYR:OH	2.13	0.49
1:A:124:ILE:HD12	1:A:140:ALA:O	2.13	0.49
2:B:65:LEU:C	2:B:65:LEU:HD23	2.38	0.48
5:E:54:ILE:HG12	5:E:55:ALA:H	1.77	0.48
4:D:211:PRO:O	4:D:214:THR:OG1	2.30	0.48
1:A:51:TRP:CZ3	1:A:52:ILE:HD13	2.46	0.48
1:A:64:THR:O	1:A:68:LYS:HB2	2.13	0.48
4:D:140:LEU:N	4:D:140:LEU:HD12	2.28	0.48
4:D:207:ASN:ND2	4:D:207:ASN:N	2.61	0.48
1:A:22:PHE:H	1:A:38:SER:HB3	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:28:VAL:HG23	1:A:33:PHE:CE2	2.48	0.48
1:A:256:ARG:HD2	1:A:256:ARG:O	2.14	0.48
4:D:11:LEU:HD13	4:D:124:LEU:HD13	1.94	0.48
1:A:178:THR:HA	1:A:239:ARG:NH2	2.28	0.48
2:B:70:PHE:HD1	2:B:78:TYR:CE2	2.32	0.48
5:E:103:PHE:CE1	5:E:118:GLY:HA3	2.49	0.48
1:A:272:LEU:HD12	1:A:272:LEU:O	2.14	0.47
1:A:228:THR:HG23	1:A:246:ALA:O	2.15	0.47
5:E:100:ALA:HA	5:E:120:ARG:NH2	2.29	0.47
1:A:97:ARG:HH21	1:A:114:ASP:CG	2.22	0.47
5:E:101:LEU:HG	5:E:120:ARG:HG2	1.97	0.47
1:A:268:LYS:HE3	1:A:268:LYS:HB2	1.69	0.47
1:A:15:PRO:O	1:A:17:ARG:HG2	2.14	0.47
5:E:107:SER:O	5:E:108:ALA:HB3	2.14	0.47
4:D:98:ASP:O	4:D:124:LEU:HD23	2.15	0.47
5:E:54:ILE:HG12	5:E:55:ALA:N	2.30	0.47
1:A:165:VAL:O	1:A:166:GLU:C	2.58	0.46
5:E:10:HIS:CD2	5:E:225:TYR:CE1	3.03	0.46
1:A:28:VAL:O	1:A:29:ASP:HB2	2.15	0.46
4:D:4:VAL:O	4:D:119:GLY:HA2	2.15	0.46
4:D:171:TYR:HE1	5:E:189:GLU:HA	1.79	0.46
1:A:7:TYR:O	1:A:98:MET:HA	2.15	0.46
2:B:35:ILE:O	2:B:83:ASN:O	2.33	0.46
1:A:81:LEU:HD12	1:A:84:TYR:CE2	2.51	0.46
1:A:187:THR:HG21	1:A:270:LEU:HD13	1.98	0.46
1:A:218:GLN:HG2	1:A:222:GLU:O	2.15	0.46
4:D:69:LYS:HA	4:D:69:LYS:HD2	1.71	0.46
5:E:4:VAL:HG21	5:E:114:PHE:O	2.15	0.46
5:E:182:THR:HB	5:E:202:SER:HB2	1.97	0.46
5:E:96:LEU:HD23	5:E:123:VAL:O	2.15	0.46
1:A:138:THR:HA	1:A:141:GLN:CD	2.40	0.46
1:A:177:GLU:O	1:A:181:ARG:NE	2.49	0.46
5:E:131:PHE:HA	5:E:132:PRO:HD3	1.77	0.46
1:A:209:TYR:CD1	1:A:210:PRO:HA	2.50	0.45
4:D:39:LEU:C	4:D:39:LEU:HD23	2.40	0.45
1:A:5:MET:O	1:A:100:GLY:HA3	2.16	0.45
1:A:28:VAL:HG23	1:A:33:PHE:CD2	2.51	0.45
1:A:203:CYS:O	1:A:244:TRP:HB2	2.16	0.45
5:E:237:ARG:NH1	5:E:240:PRO:HG3	2.29	0.45
1:A:95:ILE:C	1:A:95:ILE:HD12	2.41	0.45
5:E:57:TYR:HD2	5:E:58:ASN:N	2.14	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:244:ILE:O	5:E:244:ILE:HG13	2.15	0.45
1:A:71:THR:O	1:A:75:ARG:HG3	2.17	0.45
1:A:200:THR:HG22	1:A:202:ARG:NH2	2.31	0.45
3:C:8:TYR:CE1	5:E:108:ALA:HB2	2.51	0.45
5:E:164:HIS:HB3	5:E:225:TYR:HB2	1.99	0.45
1:A:253:GLU:H	1:A:256:ARG:HH21	1.65	0.45
4:D:83:LEU:HD22	4:D:84:THR:O	2.17	0.45
2:B:22:PHE:CZ	2:B:69:GLU:HG2	2.51	0.45
1:A:234:ARG:NE	1:A:242:GLN:HE21	2.07	0.44
4:D:13:LEU:HD22	4:D:124:LEU:HD13	2.00	0.44
4:D:149:SER:O	4:D:150:VAL:O	2.34	0.44
4:D:67:LYS:O	4:D:68:GLU:C	2.61	0.44
5:E:3:GLY:HA3	5:E:26:ARG:CG	2.37	0.44
5:E:75:ARG:HD2	5:E:92:SER:O	2.16	0.44
1:A:232:GLU:HG2	1:A:233:THR:N	2.33	0.44
2:B:5:PRO:CA	2:B:30:PHE:HB3	2.47	0.44
4:D:66:GLU:HB3	4:D:80:LYS:HE2	1.98	0.44
4:D:149:SER:O	4:D:150:VAL:HG12	2.17	0.44
5:E:170:TRP:CE3	5:E:173:GLY:O	2.71	0.44
3:C:1:HIS:ND1	3:C:2:PRO:HD2	2.33	0.44
2:B:77:GLU:CD	2:B:94:LYS:HE2	2.42	0.44
4:D:128:PRO:HG2	4:D:177:VAL:HG21	2.00	0.44
1:A:51:TRP:CE3	1:A:51:TRP:C	2.95	0.44
1:A:63:ASN:HD22	1:A:63:ASN:N	2.16	0.44
3:C:1:HIS:HA	3:C:2:PRO:HD3	1.76	0.44
1:A:15:PRO:O	1:A:17:ARG:N	2.51	0.44
1:A:232:GLU:HG2	1:A:233:THR:H	1.81	0.44
4:D:25:TYR:C	4:D:25:TYR:CD1	2.96	0.44
4:D:106:VAL:HG22	4:D:107:GLN:N	2.33	0.44
5:E:239:LYS:HA	5:E:240:PRO:HD3	1.60	0.44
5:E:83:PRO:O	5:E:84:ASP:O	2.35	0.44
2:B:50:GLU:HB2	2:B:67:TYR:CE1	2.53	0.43
4:D:25:TYR:CD1	4:D:25:TYR:O	2.72	0.43
4:D:139:GLN:C	4:D:140:LEU:HD12	2.42	0.43
5:E:105:ALA:HB2	5:E:115:PHE:CD2	2.54	0.43
1:A:156:LEU:O	1:A:160:LEU:HG	2.18	0.43
4:D:68:GLU:HB3	4:D:69:LYS:CB	2.45	0.43
2:B:65:LEU:CD2	2:B:67:TYR:HD2	2.30	0.43
4:D:140:LEU:O	4:D:149:SER:O	2.35	0.43
1:A:212:GLU:O	1:A:263:HIS:CD2	2.71	0.43
2:B:89:GLN:HG3	2:B:91:LYS:HZ2	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:14:ARG:C	1:A:17:ARG:HG3	2.43	0.43
1:A:202:ARG:HG2	1:A:204:TRP:CE2	2.54	0.43
5:E:46:LEU:HG	5:E:120:ARG:HH21	1.83	0.43
1:A:233:THR:OG1	1:A:243:LYS:HD2	2.19	0.43
5:E:194:ASN:C	5:E:196:SER:N	2.66	0.43
1:A:163:LEU:HD23	1:A:167:TRP:HE1	1.83	0.43
1:A:234:ARG:HB2	1:A:235:PRO:HD2	2.01	0.43
1:A:51:TRP:C	1:A:51:TRP:HE3	2.27	0.43
1:A:260:HIS:HA	1:A:270:LEU:O	2.19	0.43
5:E:57:TYR:HD2	5:E:58:ASN:HB2	1.80	0.43
5:E:57:TYR:HD2	5:E:58:ASN:H	1.67	0.43
1:A:14:ARG:O	1:A:15:PRO:C	2.62	0.42
4:D:180:MET:HG3	4:D:185:PHE:HD2	1.83	0.42
4:D:23:CYS:O	4:D:86:GLU:CB	2.65	0.42
5:E:68:LYS:CG	5:E:71:ILE:HD11	2.47	0.42
1:A:167:TRP:HB3	1:A:171:TYR:CE2	2.54	0.42
4:D:148:LYS:O	4:D:150:VAL:N	2.52	0.42
4:D:160:THR:HG21	4:D:211:PRO:HG3	2.00	0.42
5:E:81:PHE:HE2	5:E:88:GLU:HB2	1.83	0.42
5:E:228:SER:O	5:E:229:GLU:C	2.62	0.42
2:B:41:LYS:HE2	2:B:41:LYS:HB3	1.86	0.42
4:D:105:ALA:CB	4:D:116:LEU:HD22	2.46	0.42
5:E:30:LEU:O	5:E:57:TYR:O	2.38	0.42
5:E:130:VAL:HG12	5:E:240:PRO:CB	2.49	0.42
1:A:2:SER:CB	1:A:104:GLY:O	2.67	0.42
1:A:179:LEU:HD23	1:A:179:LEU:HA	1.89	0.42
1:A:147:TRP:NE1	3:C:10:GLU:O	2.41	0.42
1:A:90:ALA:HA	1:A:91:GLY:HA3	1.76	0.42
4:D:178:LEU:HD12	4:D:178:LEU:N	2.34	0.42
5:E:51[A]:GLN:HE21	5:E:51[A]:GLN:HB2	1.46	0.42
5:E:153:LEU:HD12	5:E:153:LEU:N	2.35	0.42
5:E:80:GLN:HE21	5:E:85:LEU:HA	1.85	0.41
1:A:183:ASP:HA	1:A:184:PRO:HD3	1.81	0.41
2:B:30:PHE:CE1	2:B:35:ILE:HD13	2.55	0.41
4:D:27:VAL:HG11	4:D:30:LEU:HB2	2.02	0.41
1:A:162:GLY:O	1:A:163:LEU:C	2.64	0.41
1:A:200:THR:HG23	1:A:248:VAL:CG2	2.50	0.41
4:D:159:GLN:NE2	7:D:222:HOH:O	2.53	0.41
5:E:6:GLN:HE21	5:E:6:GLN:HB3	1.69	0.41
5:E:75:ARG:CD	5:E:93:SER:HB2	2.42	0.41
1:A:176:LYS:O	1:A:177:GLU:HG2	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:194:VAL:O	1:A:194:VAL:HG22	2.20	0.41
1:A:260:HIS:NE2	1:A:271:THR:CG2	2.84	0.41
4:D:141:ARG:O	4:D:141:ARG:HG3	2.19	0.41
1:A:12:MET:HE2	1:A:12:MET:HB3	1.88	0.41
4:D:7:SER:O	4:D:9:GLU:N	2.53	0.41
4:D:150:VAL:O	4:D:150:VAL:CG1	2.64	0.41
5:E:30:LEU:HA	5:E:85:LEU:HD22	2.03	0.41
1:A:82:ARG:HA	1:A:87:GLN:OE1	2.21	0.41
1:A:202:ARG:HG2	1:A:204:TRP:CZ2	2.55	0.41
2:B:22:PHE:N	2:B:22:PHE:CD2	2.89	0.41
4:D:185:PHE:CE2	4:D:187:SER:HB3	2.56	0.41
5:E:127:LEU:HD13	5:E:227:LEU:HG	2.03	0.41
5:E:213:ASN:O	5:E:216:ASN:HB2	2.21	0.41
1:A:35:ARG:HD3	1:A:48:ARG:NH2	2.36	0.41
1:A:36:PHE:CD2	1:A:36:PHE:C	2.99	0.41
1:A:101:CYS:HB2	1:A:109:LEU:HD23	2.03	0.41
2:B:39:LEU:CB	2:B:46:ILE:HG21	2.50	0.41
2:B:44:GLU:HA	2:B:81:ARG:HH12	1.86	0.41
5:E:52:PHE:CD1	5:E:69:GLY:HA3	2.56	0.40
1:A:213:ILE:HG13	1:A:263:HIS:HB2	2.02	0.40
5:E:56:TYR:CD2	5:E:56:TYR:N	2.89	0.40
1:A:192:HIS:HA	1:A:193:PRO:HD3	1.91	0.40
2:B:65:LEU:HD21	2:B:67:TYR:HD2	1.86	0.40
5:E:175:GLU:OE2	7:E:261:HOH:O	2.22	0.40
1:A:117:ALA:HA	1:A:121:LYS:O	2.22	0.40
1:A:160:LEU:HA	1:A:160:LEU:HD23	1.84	0.40
1:A:236:ALA:HB3	1:A:240:THR:OG1	2.21	0.40
2:B:41:LYS:C	2:B:43:GLY:N	2.78	0.40
5:E:194:ASN:O	5:E:196:SER:N	2.55	0.40
1:A:145:ARG:HG3	1:A:145:ARG:NH1	2.19	0.40
5:E:237:ARG:HH12	5:E:240:PRO:CG	2.30	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	274/276 (99%)	229 (84%)	39 (14%)	6 (2%)	5	15
2	B	98/100 (98%)	87 (89%)	9 (9%)	2 (2%)	6	16
3	C	9/11 (82%)	8 (89%)	1 (11%)	0	100	100
4	D	199/200 (100%)	166 (83%)	23 (12%)	10 (5%)	1	3
5	E	240/241 (100%)	209 (87%)	21 (9%)	10 (4%)	2	5
All	All	820/828 (99%)	699 (85%)	93 (11%)	28 (3%)	3	7

All (28) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	15	PRO
2	B	46	ILE
4	D	68	GLU
4	D	175	LYS
4	D	194	SER
5	E	60	GLU
5	E	74	GLU
5	E	84	ASP
5	E	108	ALA
5	E	229	GLU
1	A	16	GLY
1	A	216	THR
1	A	256	ARG
4	D	150	VAL
4	D	201	CYS
5	E	195	ASP
2	B	1	ILE
4	D	149	SER
5	E	46	LEU
5	E	85	LEU
1	A	254	GLU
4	D	70	GLU
4	D	108	ASP
1	A	40	ALA
4	D	7	SER
4	D	59	ALA
5	E	100	ALA
5	E	118	GLY

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	234/234 (100%)	212 (91%)	22 (9%)	7	18
2	B	95/95 (100%)	79 (83%)	16 (17%)	1	4
3	C	9/9 (100%)	9 (100%)	0	100	100
4	D	179/178 (101%)	149 (83%)	30 (17%)	1	4
5	E	209/208 (100%)	183 (88%)	26 (12%)	4	9
All	All	726/724 (100%)	632 (87%)	94 (13%)	3	8

All (94) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	SER
1	A	42	SER
1	A	45	THR
1	A	54	GLN
1	A	81	LEU
1	A	95	ILE
1	A	109	LEU
1	A	124	ILE
1	A	131	SER
1	A	143	THR
1	A	145	ARG
1	A	146	LYS
1	A	163	LEU
1	A	177	GLU
1	A	186	LYS
1	A	187	THR
1	A	248	VAL
1	A	254	GLU
1	A	261	VAL
1	A	262	GLN
1	A	271	THR
1	A	274	TRP
2	B	0	MET

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Mol	Chain	Res	Type
2	B	1	ILE
2	B	4	THR
2	B	6	LYS
2	B	27	VAL
2	B	31	HIS
2	B	40	LEU
2	B	46	ILE
2	B	49	VAL
2	B	58	LYS
2	B	65	LEU
2	B	70	PHE
2	B	73	THR
2	B	75	LYS
2	B	88	SER
2	B	97	ARG
4	D	11	LEU
4	D	12	ARG
4	D	13	LEU
4	D	21	LEU
4	D	27	VAL
4	D	48	LYS
4	D	55	THR
4	D	58	SER
4	D	68	GLU
4	D	82	THR
4	D	83	LEU
4	D	0(A)	LYS
4	D	91	ILE
4	D	92	THR
4	D	99	SER
4	D	101	THR
4	D	109	LEU
4	D	111	THR
4	D	114	SER
4	D	115	ARG
4	D	126	VAL
4	D	150	VAL
4	D	151	CYS
4	D	154	THR
4	D	160	THR
4	D	173	THR
4	D	177	VAL

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Mol	Chain	Res	Type
4	D	180	MET
4	D	207	ASN
4	D	210	ILE
5	E	23	CYS
5	E	26	ARG
5	E	46	LEU
5	E	51[A]	GLN
5	E	51[B]	GLN
5	E	66[A]	ARG
5	E	71	ILE
5	E	74	GLU
5	E	104	CYS
5	E	110	SER
5	E	112	GLU
5	E	113	LEU
5	E	117	GLU
5	E	119	SER
5	E	120	ARG
5	E	152	THR
5	E	156	LEU
5	E	164	HIS
5	E	166	GLU
5	E	180	VAL
5	E	182	THR
5	E	190	GLN
5	E	221	GLN
5	E	227	LEU
5	E	242	THR
5	E	246	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	63	ASN
1	A	65	GLN
1	A	93	HIS
1	A	174	ASN
1	A	192	HIS
1	A	218	GLN
1	A	242	GLN
1	A	263	HIS
2	B	2	GLN

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Mol	Chain	Res	Type
2	B	24	ASN
2	B	42	ASN
4	D	14	GLN
4	D	44	GLN
4	D	129	ASN
4	D	159	GLN
4	D	207	ASN
5	E	43	GLN
5	E	44	GLN
5	E	86	HIS
5	E	164	HIS
5	E	177	HIS
5	E	185	GLN
5	E	190	GLN
5	E	212	GLN
5	E	213	ASN
5	E	216	ASN
5	E	221	GLN
5	E	223	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

1 ligand is 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	$\# Z > 2$
6	SO4	D	1	-	4,4,4	0.24	0	6,6,6	0.07	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	276/276 (100%)	1.04	50 (18%) 4 4	21, 48, 116, 132	0
2	B	100/100 (100%)	1.18	14 (14%) 7 7	38, 67, 91, 99	0
3	C	11/11 (100%)	-0.06	0 100 100	21, 24, 28, 30	0
4	D	200/200 (100%)	0.30	4 (2%) 64 64	13, 31, 67, 90	1 (0%)
5	E	241/241 (100%)	0.30	2 (0%) 82 82	12, 34, 65, 90	1 (0%)
All	All	828/828 (100%)	0.65	70 (8%) 18 17	12, 39, 101, 132	2 (0%)

All (70) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	190	THR	5.2
1	A	249	VAL	4.5
1	A	217	TRP	4.4
1	A	257	TYR	4.4
1	A	258	THR	4.3
1	A	250	PRO	4.1
1	A	272	LEU	4.0
1	A	228	THR	3.9
1	A	247	VAL	3.6
1	A	194	VAL	3.5
1	A	193	PRO	3.4
1	A	211	ALA	3.4
1	A	189	VAL	3.3
2	B	55	SER	3.3
1	A	195	SER	3.2
1	A	199	ALA	3.1
2	B	92	ILE	3.1
1	A	261	VAL	3.0
2	B	79	ALA	3.0
1	A	248	VAL	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	227	ASP	2.9
2	B	46	ILE	2.9
1	A	203	CYS	2.9
2	B	43	GLY	2.9
2	B	71	THR	2.9
1	A	187	THR	2.8
1	A	260	HIS	2.8
5	E	46	LEU	2.8
1	A	229	GLU	2.8
4	D	7	SER	2.8
1	A	274	TRP	2.8
1	A	275	GLU	2.7
1	A	213	ILE	2.7
1	A	216	THR	2.7
2	B	93	VAL	2.6
5	E	71	ILE	2.6
4	D	182	SER	2.5
2	B	39	LEU	2.5
1	A	256	ARG	2.5
1	A	197	HIS	2.5
1	A	200	THR	2.5
1	A	259	CYS	2.5
4	D	201	CYS	2.4
1	A	226	GLN	2.4
1	A	15	PRO	2.4
1	A	20	PRO	2.4
1	A	184	PRO	2.4
1	A	276	PRO	2.3
2	B	0	MET	2.3
2	B	41	LYS	2.3
1	A	204	TRP	2.3
1	A	254	GLU	2.3
1	A	188	HIS	2.3
1	A	245	ALA	2.3
2	B	40	LEU	2.3
1	A	266	LEU	2.2
1	A	251	SER	2.1
1	A	273	ARG	2.1
1	A	231	VAL	2.1
2	B	38	ASP	2.1
1	A	19	GLU	2.1
1	A	186	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	26	GLY	2.1
1	A	201	LEU	2.1
1	A	221	GLY	2.1
1	A	269	PRO	2.0
2	B	72	PRO	2.0
1	A	263	HIS	2.0
2	B	24	ASN	2.0
4	D	47	GLY	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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(\AA^2)	Q<0.9
6	SO4	D	1	5/5	0.72	0.22	72,87,99,109	0

6.5 Other polymers [i](#)

There are no such residues in this entry.