



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:03 AM UTC

PDB ID : 1IAS / pdb_00001ias
Title : CYTOPLASMIC DOMAIN OF UNPHOSPHORYLATED TYPE I TGF-BETA RECEPTOR CRYSTALLIZED WITHOUT FKBP12
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Deposited on : 2001-03-23
Resolution : 2.90 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

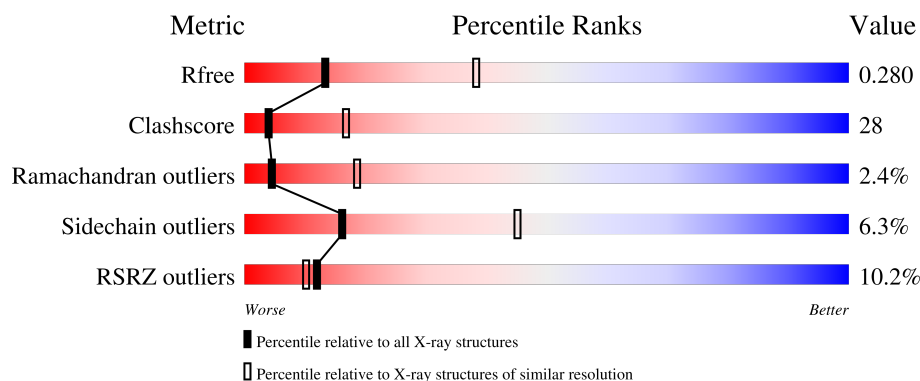
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	342	8% 51% 38% 8%
1	B	342	7% 50% 38% 7% 5%
1	C	342	15% 48% 41% 8%
1	D	342	11% 51% 37% 8%
1	E	342	8% 51% 37% 8%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SO4	E	1	-	-	X	-

2 Entry composition [i](#)

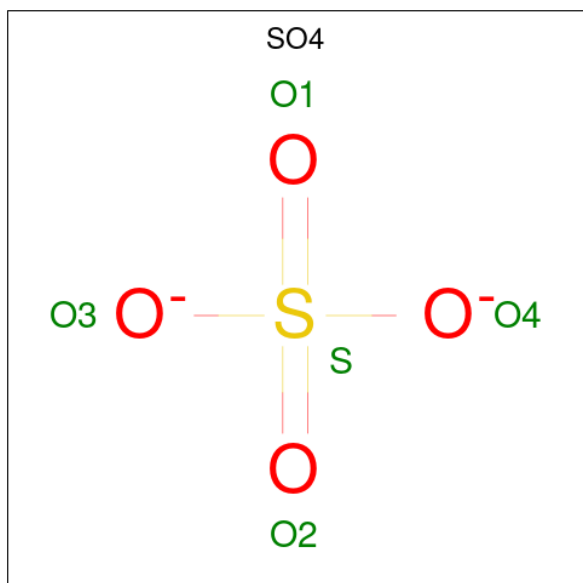
There are 2 unique types of molecules in this entry. The entry contains 13181 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 TGF-BETA RECEPTOR TYPE I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	330	Total	C	N	O	S	0	0	0
			2629	1658	471	484	16			
1	B	324	Total	C	N	O	S	0	0	0
			2590	1636	463	475	16			
1	C	330	Total	C	N	O	S	0	0	0
			2629	1658	471	484	16			
1	D	330	Total	C	N	O	S	0	0	0
			2629	1658	471	484	16			
1	E	330	Total	C	N	O	S	0	0	0
			2629	1658	471	484	16			

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

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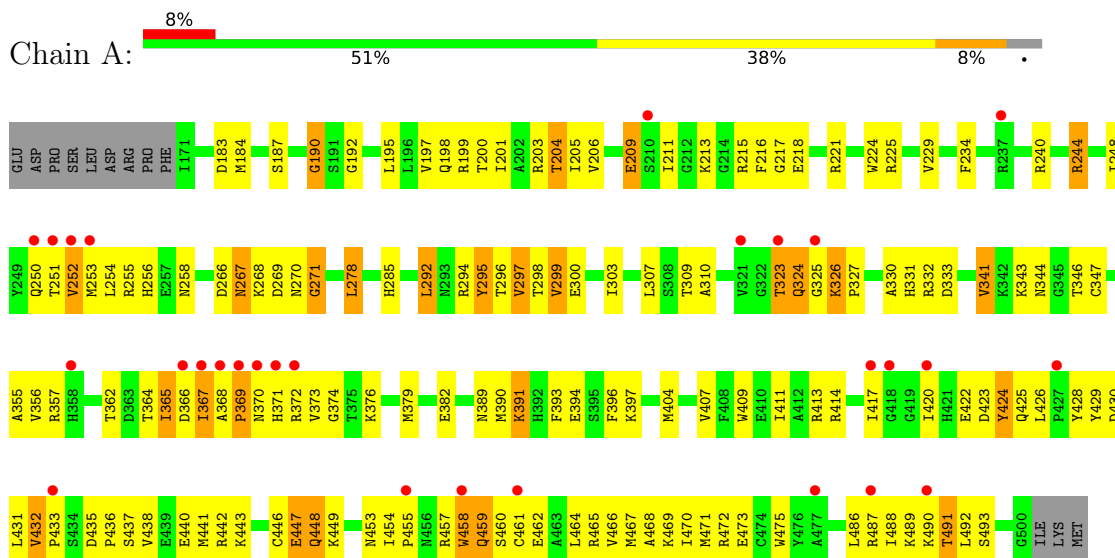
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0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

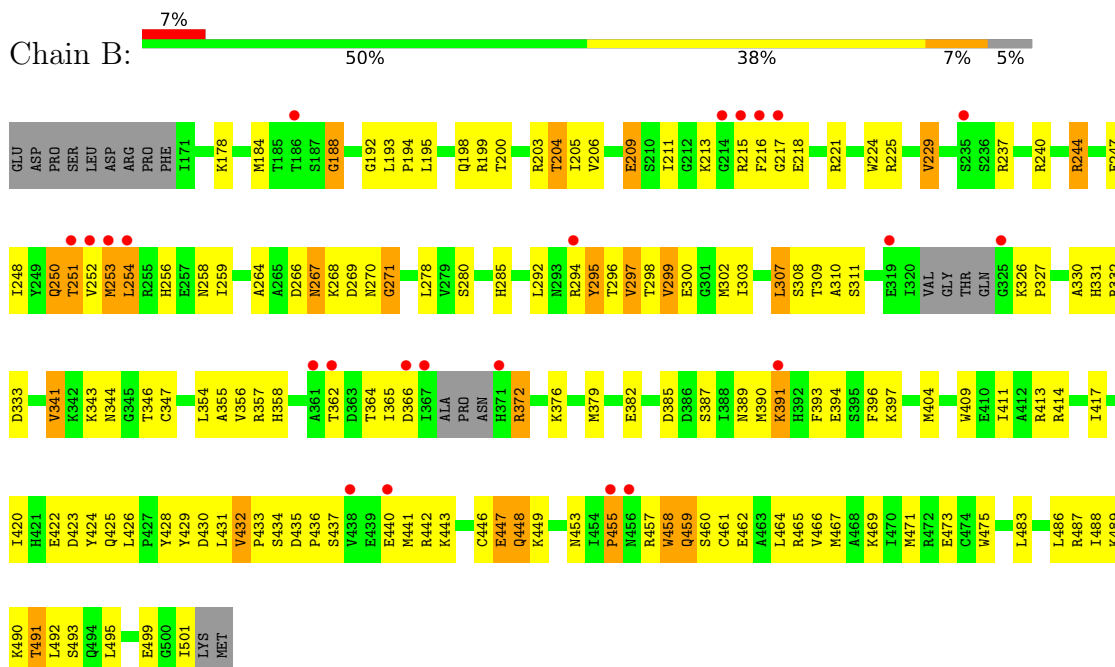
3 Residue-property plots

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.

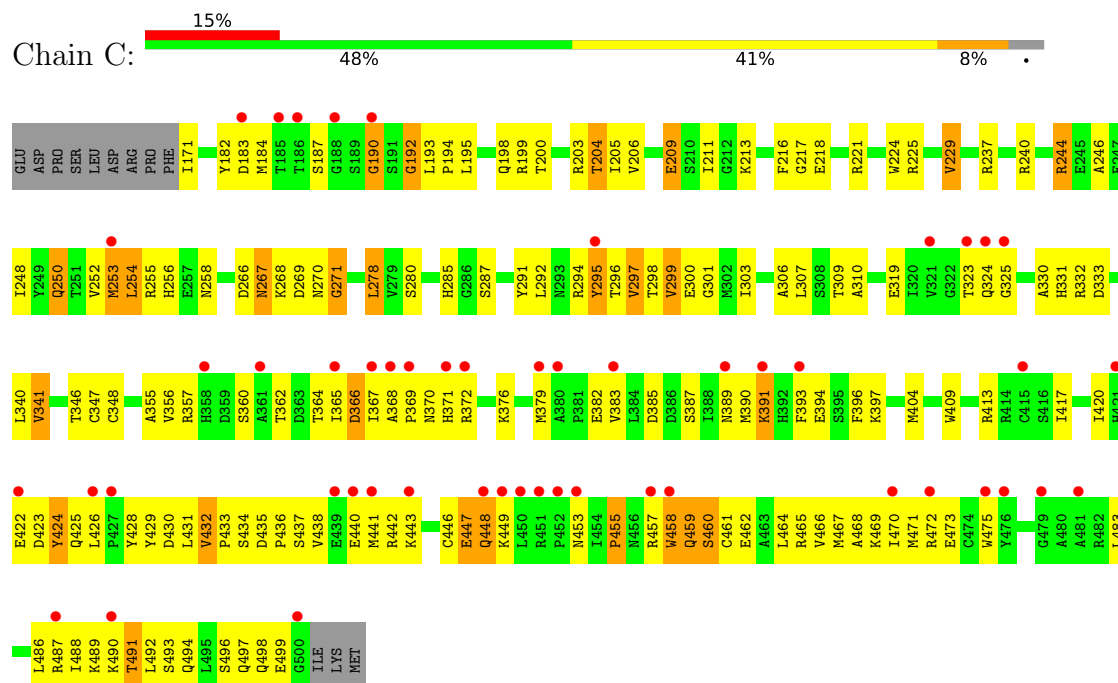
• Molecule 1: TGF-BETA RECEPTOR TYPE I

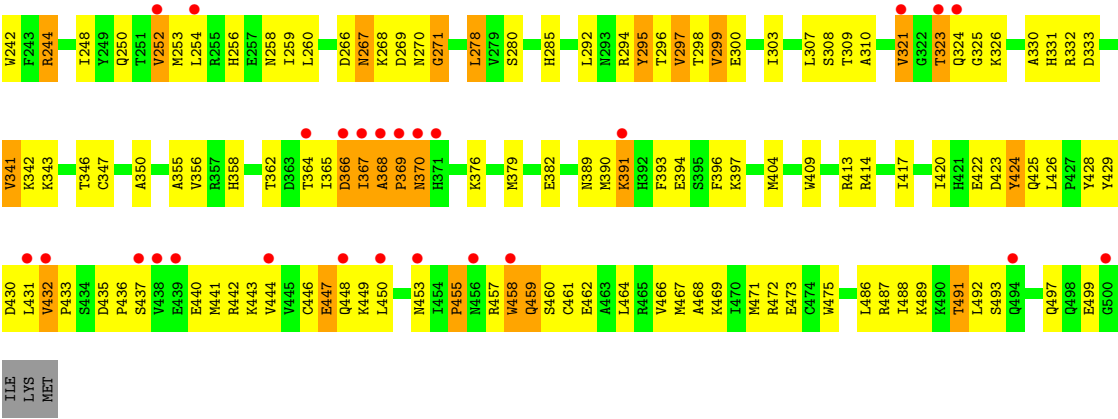


• Molecule 1: TGF-BETA RECEPTOR TYPE I



• Molecule 1: TGF-BETA RECEPTOR TYPE I





ILE
LYS
MET

4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	172.56Å 251.62Å 140.23Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.90 30.00 – 2.91	Depositor EDS
% Data completeness (in resolution range)	85.9 (30.00-2.90) 85.9 (30.00-2.91)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.81 (at 2.91Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.255 , 0.284 0.254 , 0.280	Depositor DCC
R_{free} test set	6041 reflections (10.14%)	wwPDB-VP
Wilson B-factor (Å ²)	56.3	Xtriage
Anisotropy	0.740	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 42.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	13181	wwPDB-VP
Average B, all atoms (Å ²)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.21% 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	0.50	0/2682	0.98	11/3622 (0.3%)
1	B	0.53	0/2640	0.97	11/3560 (0.3%)
1	C	0.48	0/2682	0.97	11/3622 (0.3%)
1	D	0.53	0/2682	1.02	14/3622 (0.4%)
1	E	0.55	0/2682	1.01	13/3622 (0.4%)
All	All	0.52	0/13368	0.99	60/18048 (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	A	0	1
1	C	0	1
1	D	0	1
1	E	0	1
All	All	0	4

There are no bond length outliers.

All (60) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	321	VAL	N-CA-C	9.76	125.70	112.04
1	E	252	VAL	N-CA-C	8.28	121.15	113.20
1	B	296	THR	N-CA-C	-7.64	97.80	109.41
1	D	296	THR	N-CA-C	-7.37	98.21	109.41
1	A	296	THR	N-CA-C	-7.14	98.56	109.41
1	E	296	THR	N-CA-C	-7.12	98.58	109.41
1	B	253	MET	N-CA-C	-7.08	101.47	111.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	296	THR	N-CA-C	-7.06	98.67	109.41
1	E	268	LYS	N-CA-C	6.99	125.68	110.80
1	E	324	GLN	N-CA-C	-6.88	104.76	113.02
1	A	190	GLY	N-CA-C	-6.79	104.93	115.73
1	D	268	LYS	N-CA-C	6.67	125.00	110.80
1	B	268	LYS	N-CA-C	6.63	124.92	110.80
1	A	268	LYS	N-CA-C	6.62	124.90	110.80
1	C	268	LYS	N-CA-C	6.50	124.64	110.80
1	D	367	ILE	N-CA-C	6.44	116.67	108.82
1	D	432	VAL	CA-C-N	6.30	126.66	119.92
1	D	432	VAL	C-N-CA	6.30	126.66	119.92
1	D	321	VAL	N-CA-C	6.29	118.95	111.09
1	B	432	VAL	CA-C-N	6.18	126.53	119.92
1	B	432	VAL	C-N-CA	6.18	126.53	119.92
1	E	432	VAL	CA-C-N	6.12	126.46	119.92
1	E	432	VAL	C-N-CA	6.12	126.46	119.92
1	A	299	VAL	N-CA-C	-6.06	104.44	110.62
1	A	391	LYS	N-CA-C	-6.01	106.10	113.50
1	E	299	VAL	N-CA-C	-6.00	104.66	110.72
1	A	432	VAL	CA-C-N	5.92	126.26	119.92
1	A	432	VAL	C-N-CA	5.92	126.26	119.92
1	C	432	VAL	CA-C-N	5.90	126.23	119.92
1	C	432	VAL	C-N-CA	5.90	126.23	119.92
1	B	299	VAL	N-CA-C	-5.84	104.67	110.62
1	B	391	LYS	N-CA-C	-5.83	106.29	113.41
1	C	391	LYS	N-CA-C	-5.79	106.34	113.41
1	E	459	GLN	N-CA-C	-5.73	106.33	113.38
1	D	297	VAL	N-CA-C	5.71	118.39	108.90
1	B	295	TYR	N-CA-C	5.68	117.25	109.18
1	A	297	VAL	N-CA-C	5.67	118.32	108.90
1	B	297	VAL	N-CA-C	5.66	118.30	108.90
1	C	297	VAL	N-CA-C	5.65	118.28	108.90
1	E	297	VAL	N-CA-C	5.63	118.25	108.90
1	C	250	GLN	N-CA-C	5.60	117.07	110.97
1	A	252	VAL	N-CA-C	5.59	117.58	111.77
1	E	391	LYS	N-CA-C	-5.58	106.64	113.50
1	C	295	TYR	N-CA-C	5.57	117.08	109.18
1	D	391	LYS	N-CA-C	-5.53	106.67	113.41
1	D	295	TYR	N-CA-C	5.49	116.98	109.18
1	C	192	GLY	N-CA-C	-5.47	102.92	112.55
1	D	499	GLU	N-CA-CB	5.41	119.91	111.64
1	E	295	TYR	N-CA-C	5.37	116.80	109.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	324	GLN	N-CA-C	-5.32	106.77	113.20
1	C	299	VAL	N-CA-C	-5.31	105.20	110.62
1	D	459	GLN	N-CA-C	-5.31	106.85	113.38
1	C	459	GLN	N-CA-C	-5.28	106.89	113.38
1	D	299	VAL	N-CA-C	-5.22	105.30	110.62
1	A	459	GLN	N-CA-C	-5.19	106.99	113.38
1	B	250	GLN	N-CA-C	5.16	116.59	110.97
1	E	370	ASN	N-CA-C	5.13	119.26	113.15
1	B	459	GLN	N-CA-C	-5.09	107.08	113.28
1	A	295	TYR	N-CA-C	5.06	116.37	109.18
1	D	499	GLU	CB-CA-C	-5.03	103.74	111.74

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	424	TYR	Sidechain
1	C	424	TYR	Sidechain
1	D	424	TYR	Sidechain
1	E	424	TYR	Sidechain

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	2629	0	2631	146	0
1	B	2590	0	2595	137	0
1	C	2629	0	2631	158	0
1	D	2629	0	2631	155	0
1	E	2629	0	2631	148	1
2	A	15	0	0	1	0
2	B	15	0	0	1	0
2	C	15	0	0	0	0
2	D	15	0	0	0	0
2	E	15	0	0	2	0
All	All	13181	0	13119	737	1

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 28.

All (737) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:191:SER:HB2	1:E:253:MET:HA	1.31	1.12
1:E:368:ALA:HB3	1:E:369:PRO:HD3	1.37	1.05
1:A:298:THR:HG22	1:A:300:GLU:H	1.26	1.00
1:B:298:THR:HG22	1:B:300:GLU:H	1.27	0.98
1:C:298:THR:HG22	1:C:300:GLU:H	1.27	0.96
1:B:309:THR:HG22	1:B:404:MET:HE2	1.43	0.96
1:D:368:ALA:HB2	1:E:178:LYS:HE2	1.44	0.95
1:E:298:THR:HG22	1:E:300:GLU:H	1.26	0.95
1:A:332:ARG:NH2	1:A:369:PRO:HG2	1.82	0.94
1:E:309:THR:HG22	1:E:404:MET:HE2	1.50	0.94
1:E:211:ILE:HD11	1:E:221:ARG:HB2	1.50	0.94
1:C:309:THR:HG22	1:C:404:MET:HE2	1.50	0.93
1:E:368:ALA:CB	1:E:369:PRO:HD3	1.99	0.92
1:D:298:THR:HG22	1:D:300:GLU:H	1.30	0.91
1:C:211:ILE:HD11	1:C:221:ARG:HB2	1.51	0.91
1:D:267:ASN:H	1:D:267:ASN:HD22	1.21	0.89
1:A:372:ARG:HG2	1:A:379:MET:HE1	1.54	0.88
1:D:211:ILE:HD11	1:D:221:ARG:HB2	1.54	0.88
1:A:309:THR:HG22	1:A:404:MET:HE2	1.53	0.88
1:B:211:ILE:HD11	1:B:221:ARG:HB2	1.55	0.87
1:D:309:THR:HG22	1:D:404:MET:HE2	1.54	0.87
1:C:372:ARG:NH2	1:C:438:VAL:HG11	1.90	0.86
1:E:191:SER:HB2	1:E:253:MET:CA	2.04	0.86
1:B:443:LYS:HG2	1:B:448:GLN:HE21	1.39	0.86
1:D:252:VAL:O	1:D:253:MET:HG2	1.74	0.86
1:A:211:ILE:HD11	1:A:221:ARG:HB2	1.57	0.86
1:D:443:LYS:HG2	1:D:448:GLN:HE21	1.41	0.86
1:A:332:ARG:HH22	1:A:369:PRO:HG2	1.40	0.86
1:C:372:ARG:HH22	1:C:438:VAL:HG11	1.38	0.86
1:E:443:LYS:HG2	1:E:448:GLN:HE21	1.40	0.86
1:A:443:LYS:HG2	1:A:448:GLN:HE21	1.38	0.85
1:C:443:LYS:HG2	1:C:448:GLN:HE21	1.42	0.85
1:E:204:THR:CG2	1:E:224:TRP:HE1	1.90	0.85
1:A:267:ASN:HD22	1:A:267:ASN:H	1.25	0.83
1:B:178:LYS:HE2	1:C:369:PRO:CD	2.09	0.83
1:B:267:ASN:H	1:B:267:ASN:HD22	1.27	0.82
1:D:252:VAL:HG13	1:D:326:LYS:HB2	1.61	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:184:MET:HE2	1:A:255:ARG:NH1	1.94	0.81
1:C:204:THR:CG2	1:C:224:TRP:HE1	1.93	0.81
1:E:332:ARG:NH2	1:E:369:PRO:HD2	1.95	0.81
1:C:267:ASN:HD22	1:C:267:ASN:H	1.26	0.81
1:E:298:THR:HG22	1:E:300:GLU:N	1.96	0.80
1:B:178:LYS:HE2	1:C:369:PRO:HD3	1.63	0.80
1:A:298:THR:HG22	1:A:300:GLU:N	1.97	0.80
1:B:204:THR:CG2	1:B:224:TRP:HE1	1.96	0.79
1:C:298:THR:HG22	1:C:300:GLU:N	1.97	0.79
1:A:372:ARG:NH1	1:A:438:VAL:HG11	1.98	0.79
1:B:298:THR:HG22	1:B:300:GLU:N	1.97	0.79
1:C:199:ARG:HD2	1:C:203:ARG:CZ	2.13	0.79
1:E:267:ASN:HD22	1:E:267:ASN:H	1.27	0.79
1:A:204:THR:CG2	1:A:224:TRP:HE1	1.96	0.78
1:D:204:THR:CG2	1:D:224:TRP:HE1	1.96	0.78
1:A:368:ALA:HB3	1:A:369:PRO:HD3	1.66	0.78
1:C:182:TYR:CD1	1:E:366:ASP:HB2	2.18	0.78
1:E:199:ARG:HD2	1:E:203:ARG:CZ	2.12	0.78
1:E:368:ALA:HB3	1:E:369:PRO:CD	2.14	0.78
1:D:256:HIS:CD2	1:D:258:ASN:H	2.03	0.76
1:E:256:HIS:CD2	1:E:258:ASN:H	2.02	0.76
1:B:199:ARG:HD2	1:B:203:ARG:CZ	2.15	0.76
1:C:256:HIS:CD2	1:C:258:ASN:H	2.03	0.76
1:D:294:ARG:HD2	1:D:295:TYR:CE1	2.21	0.76
1:D:365:ILE:HG23	1:D:367:ILE:H	1.51	0.76
1:C:368:ALA:HB3	1:C:369:PRO:HD3	1.68	0.76
1:B:256:HIS:CD2	1:B:258:ASN:H	2.05	0.75
1:D:199:ARG:HD2	1:D:203:ARG:CZ	2.16	0.75
1:D:298:THR:HG22	1:D:300:GLU:N	1.99	0.75
1:A:256:HIS:CD2	1:A:258:ASN:H	2.03	0.75
1:B:409:TRP:HB2	1:B:471:MET:HE3	1.68	0.75
1:E:310:ALA:HA	1:E:404:MET:HE1	1.68	0.75
1:B:310:ALA:HA	1:B:404:MET:HE1	1.67	0.74
1:E:332:ARG:HH22	1:E:369:PRO:HD2	1.53	0.74
1:C:409:TRP:HB2	1:C:471:MET:HE3	1.69	0.74
1:B:294:ARG:HD2	1:B:295:TYR:CE1	2.22	0.74
1:C:252:VAL:O	1:C:253:MET:HB3	1.88	0.74
1:C:294:ARG:HD2	1:C:295:TYR:CE1	2.23	0.74
1:D:417:ILE:O	1:D:420:ILE:HG12	1.88	0.73
1:B:417:ILE:O	1:B:420:ILE:HG12	1.88	0.73
1:E:417:ILE:O	1:E:420:ILE:HG12	1.89	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:267:ASN:HD22	1:D:267:ASN:N	1.85	0.73
1:A:294:ARG:HD2	1:A:295:TYR:CE1	2.23	0.72
1:A:199:ARG:HD2	1:A:203:ARG:CZ	2.19	0.72
1:A:372:ARG:CG	1:A:379:MET:HE1	2.18	0.72
1:C:417:ILE:O	1:C:420:ILE:HG12	1.89	0.72
1:C:248:ILE:HD13	1:C:355:ALA:HB3	1.69	0.72
1:E:437:SER:OG	1:E:440:GLU:HG3	1.89	0.72
1:E:409:TRP:HB2	1:E:471:MET:HE3	1.71	0.72
1:B:437:SER:OG	1:B:440:GLU:HG3	1.90	0.72
1:D:409:TRP:HB2	1:D:471:MET:HE3	1.71	0.72
1:E:294:ARG:HD2	1:E:295:TYR:CE1	2.24	0.71
1:A:417:ILE:O	1:A:420:ILE:HG12	1.89	0.71
1:D:368:ALA:HB2	1:E:178:LYS:CE	2.17	0.71
1:D:244:ARG:HH22	1:D:366:ASP:CG	1.98	0.71
1:A:409:TRP:HD1	1:A:471:MET:HE1	1.56	0.71
1:C:453:ASN:O	1:C:455:PRO:HD3	1.90	0.71
1:E:184:MET:HE3	1:E:192:GLY:HA2	1.71	0.71
1:B:216:PHE:CD1	1:B:217:GLY:N	2.59	0.70
1:A:409:TRP:HB2	1:A:471:MET:HE3	1.73	0.70
1:E:453:ASN:O	1:E:455:PRO:HD3	1.91	0.70
1:A:310:ALA:HA	1:A:404:MET:HE1	1.73	0.70
1:C:437:SER:OG	1:C:440:GLU:HG3	1.90	0.70
1:D:409:TRP:HD1	1:D:471:MET:HE1	1.56	0.70
1:D:453:ASN:O	1:D:455:PRO:HD3	1.92	0.70
1:A:453:ASN:O	1:A:455:PRO:HD3	1.92	0.70
1:D:216:PHE:CD1	1:D:217:GLY:N	2.60	0.70
1:A:437:SER:OG	1:A:440:GLU:HG3	1.91	0.70
1:D:310:ALA:HA	1:D:404:MET:HE1	1.73	0.69
1:C:216:PHE:CD1	1:C:217:GLY:N	2.61	0.69
1:A:267:ASN:HD22	1:A:267:ASN:N	1.90	0.69
1:C:310:ALA:HA	1:C:404:MET:HE1	1.73	0.68
1:D:267:ASN:H	1:D:267:ASN:ND2	1.90	0.68
1:C:190:GLY:HA3	1:C:324:GLN:HE22	1.57	0.68
1:E:216:PHE:CD1	1:E:217:GLY:N	2.61	0.68
1:C:409:TRP:HD1	1:C:471:MET:HE1	1.58	0.68
1:C:461:CYS:SG	1:C:464:LEU:HD23	2.34	0.67
1:E:461:CYS:SG	1:E:464:LEU:HD23	2.34	0.67
1:A:216:PHE:CD1	1:A:217:GLY:N	2.62	0.67
1:C:371:HIS:CG	1:C:372:ARG:H	2.12	0.67
1:D:253:MET:O	1:D:253:MET:HG3	1.95	0.67
1:B:453:ASN:O	1:B:455:PRO:HD3	1.95	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:248:ILE:HD13	1:D:355:ALA:HB3	1.77	0.67
1:D:437:SER:OG	1:D:440:GLU:HG3	1.94	0.67
1:E:256:HIS:HD2	1:E:258:ASN:H	1.41	0.67
1:E:367:ILE:HG12	1:E:370:ASN:HD21	1.60	0.67
1:D:372:ARG:HD3	1:D:379:MET:HE1	1.77	0.67
1:C:365:ILE:HG22	1:C:366:ASP:N	2.10	0.67
1:C:498:GLN:O	1:C:499:GLU:HG3	1.95	0.66
1:B:267:ASN:HD22	1:B:267:ASN:N	1.92	0.66
1:A:254:LEU:HD12	1:A:255:ARG:H	1.59	0.66
1:D:357:ARG:HB2	1:D:366:ASP:HB2	1.78	0.66
1:E:409:TRP:HD1	1:E:471:MET:HE1	1.58	0.66
1:E:204:THR:CG2	1:E:224:TRP:NE1	2.59	0.65
1:D:461:CYS:SG	1:D:464:LEU:HD23	2.36	0.65
1:E:267:ASN:HD22	1:E:267:ASN:N	1.93	0.65
1:B:409:TRP:HD1	1:B:471:MET:HE1	1.61	0.65
1:C:357:ARG:H	1:C:366:ASP:HB2	1.62	0.65
1:B:365:ILE:O	1:B:365:ILE:HG13	1.95	0.65
1:B:251:THR:HG21	1:B:357:ARG:NH1	2.11	0.65
1:C:368:ALA:HB3	1:C:369:PRO:CD	2.27	0.64
1:C:285:HIS:HB2	1:C:341:VAL:O	1.97	0.64
1:D:256:HIS:HD2	1:D:258:ASN:H	1.44	0.64
1:D:365:ILE:HD11	1:D:393:PHE:HD1	1.62	0.64
1:E:184:MET:HE3	1:E:192:GLY:CA	2.26	0.64
1:E:209:GLU:OE2	1:E:221:ARG:NH1	2.28	0.64
1:A:323:THR:C	1:A:325:GLY:H	2.06	0.64
1:C:332:ARG:NH2	1:C:367:ILE:HD12	2.13	0.64
1:B:267:ASN:H	1:B:267:ASN:ND2	1.95	0.64
1:A:365:ILE:N	1:A:365:ILE:HD12	2.12	0.63
1:A:267:ASN:H	1:A:267:ASN:ND2	1.94	0.63
1:D:372:ARG:HG2	1:D:379:MET:HE1	1.79	0.63
1:A:209:GLU:OE2	1:A:221:ARG:NH1	2.27	0.63
1:C:256:HIS:HD2	1:C:258:ASN:H	1.45	0.63
1:A:256:HIS:HD2	1:A:258:ASN:H	1.43	0.63
1:E:267:ASN:H	1:E:267:ASN:ND2	1.95	0.63
1:C:267:ASN:H	1:C:267:ASN:ND2	1.95	0.63
1:A:447:GLU:O	1:A:449:LYS:HG3	1.98	0.63
1:C:447:GLU:O	1:C:449:LYS:HG3	1.99	0.63
1:A:309:THR:HG22	1:A:404:MET:CE	2.27	0.63
1:C:209:GLU:OE2	1:C:221:ARG:NH1	2.28	0.62
1:D:209:GLU:OE2	1:D:221:ARG:NH1	2.27	0.62
1:D:376:LYS:HA	1:D:379:MET:HG3	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:204:THR:CG2	1:C:224:TRP:NE1	2.63	0.62
1:E:200:THR:O	1:E:204:THR:HB	2.00	0.62
1:D:204:THR:CG2	1:D:224:TRP:NE1	2.63	0.61
1:A:409:TRP:CD1	1:A:471:MET:HE1	2.35	0.61
1:B:331:HIS:HD2	1:B:333:ASP:H	1.49	0.61
1:C:248:ILE:CD1	1:C:355:ALA:HB3	2.30	0.61
1:E:409:TRP:CD1	1:E:471:MET:HE1	2.35	0.61
1:E:447:GLU:O	1:E:449:LYS:HG3	2.01	0.61
1:B:200:THR:O	1:B:204:THR:HB	2.01	0.61
1:E:252:VAL:O	1:E:253:MET:HB3	2.01	0.61
1:B:199:ARG:HD3	1:B:266:ASP:OD2	1.99	0.61
1:D:447:GLU:O	1:D:449:LYS:HG3	2.01	0.61
1:D:409:TRP:CD1	1:D:471:MET:HE1	2.34	0.61
1:B:267:ASN:N	1:B:267:ASN:ND2	2.49	0.60
1:B:309:THR:HG22	1:B:404:MET:CE	2.26	0.60
1:E:362:THR:HG22	1:E:364:THR:HG23	1.83	0.60
1:B:461:CYS:SG	1:B:464:LEU:HD23	2.40	0.60
1:A:297:VAL:HG22	1:A:298:THR:N	2.16	0.60
1:B:447:GLU:O	1:B:449:LYS:HG3	2.02	0.60
1:E:430:ASP:OD1	1:E:431:LEU:HG	2.00	0.60
1:D:368:ALA:CB	1:E:178:LYS:HE2	2.27	0.60
1:E:244:ARG:HG2	1:E:244:ARG:HH11	1.67	0.60
1:C:409:TRP:CD1	1:C:471:MET:HE1	2.35	0.60
1:E:309:THR:HG22	1:E:404:MET:CE	2.29	0.60
1:B:297:VAL:HG22	1:B:298:THR:N	2.16	0.60
1:C:297:VAL:HG22	1:C:298:THR:N	2.17	0.60
1:B:204:THR:CG2	1:B:224:TRP:NE1	2.64	0.60
1:D:326:LYS:HB2	1:D:327:PRO:HD2	1.84	0.59
1:A:267:ASN:N	1:A:267:ASN:ND2	2.48	0.59
1:A:461:CYS:SG	1:A:464:LEU:HD23	2.42	0.59
1:B:209:GLU:OE2	1:B:221:ARG:NH1	2.29	0.59
1:E:422:GLU:N	1:E:422:GLU:OE1	2.35	0.59
1:C:498:GLN:C	1:C:499:GLU:HG3	2.28	0.59
1:B:244:ARG:HG2	1:B:244:ARG:HH11	1.67	0.59
1:B:256:HIS:HD2	1:B:258:ASN:H	1.47	0.59
1:A:204:THR:CG2	1:A:224:TRP:NE1	2.65	0.59
1:D:368:ALA:C	1:D:370:ASN:H	2.09	0.59
1:A:367:ILE:HD12	1:A:370:ASN:OD1	2.03	0.59
1:B:362:THR:HG22	1:B:364:THR:HG23	1.85	0.59
1:D:297:VAL:HG22	1:D:298:THR:N	2.18	0.59
1:E:198:GLN:HE22	1:E:250:GLN:NE2	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:369:PRO:HB2	1:A:373:VAL:HG11	1.85	0.59
1:E:204:THR:HG22	1:E:224:TRP:HE1	1.67	0.58
1:E:297:VAL:HG22	1:E:298:THR:N	2.18	0.58
1:C:244:ARG:NH2	1:C:366:ASP:HB3	2.17	0.58
1:A:430:ASP:OD1	1:A:431:LEU:HG	2.03	0.58
1:C:331:HIS:HD2	1:C:333:ASP:H	1.51	0.58
1:C:362:THR:HG22	1:C:364:THR:HG23	1.85	0.58
1:C:430:ASP:OD1	1:C:431:LEU:HG	2.04	0.58
1:B:294:ARG:HD2	1:B:295:TYR:CZ	2.38	0.58
1:B:422:GLU:N	1:B:422:GLU:OE1	2.36	0.58
1:C:182:TYR:CE1	1:E:366:ASP:HB2	2.38	0.58
1:C:365:ILE:HG22	1:C:366:ASP:H	1.67	0.58
1:E:180:LEU:HD13	1:E:201:ILE:HD11	1.86	0.58
1:E:343:LYS:HB2	2:E:1:SO4:O2	2.03	0.58
1:A:190:GLY:HA3	1:A:253:MET:SD	2.44	0.58
1:D:430:ASP:OD1	1:D:431:LEU:HG	2.03	0.57
1:A:422:GLU:OE1	1:A:422:GLU:N	2.37	0.57
1:D:200:THR:O	1:D:204:THR:HB	2.04	0.57
1:C:253:MET:O	1:C:253:MET:HG2	2.05	0.57
1:C:309:THR:HG22	1:C:404:MET:CE	2.28	0.57
1:C:422:GLU:OE1	1:C:422:GLU:N	2.38	0.57
1:A:200:THR:O	1:A:204:THR:HB	2.04	0.57
1:B:252:VAL:HG13	1:B:327:PRO:HD2	1.85	0.57
1:B:409:TRP:CD1	1:B:471:MET:HE1	2.39	0.57
1:E:248:ILE:HD13	1:E:355:ALA:HB3	1.86	0.57
1:C:200:THR:O	1:C:204:THR:HB	2.04	0.57
1:C:428:TYR:CD1	1:C:441:MET:HE1	2.40	0.57
1:A:376:LYS:HA	1:A:379:MET:HG3	1.86	0.57
1:D:253:MET:O	1:D:253:MET:CG	2.53	0.57
1:B:376:LYS:HA	1:B:379:MET:HG3	1.87	0.57
1:B:430:ASP:OD1	1:B:431:LEU:HG	2.04	0.57
1:D:199:ARG:HD3	1:D:266:ASP:OD2	2.04	0.57
1:E:331:HIS:HD2	1:E:333:ASP:H	1.52	0.57
1:B:229:VAL:HG22	1:B:280:SER:O	2.05	0.57
1:D:267:ASN:N	1:D:267:ASN:ND2	2.44	0.57
1:A:254:LEU:HD12	1:A:255:ARG:N	2.19	0.56
1:C:376:LYS:HA	1:C:379:MET:HG3	1.86	0.56
1:E:199:ARG:HD3	1:E:266:ASP:OD2	2.05	0.56
1:D:294:ARG:HD2	1:D:295:TYR:CZ	2.39	0.56
1:B:198:GLN:HE22	1:B:250:GLN:NE2	2.03	0.56
1:C:389:ASN:HD21	1:C:391:LYS:HB3	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:267:ASN:N	1:E:267:ASN:ND2	2.50	0.56
1:E:428:TYR:CD1	1:E:441:MET:HE1	2.41	0.56
1:B:258:ASN:ND2	1:B:311:SER:HB2	2.21	0.56
1:A:190:GLY:HA3	1:A:253:MET:CE	2.36	0.56
1:B:330:ALA:HB3	1:B:356:VAL:HG22	1.88	0.56
1:D:177:LEU:N	1:D:227:GLU:OE1	2.34	0.56
1:B:251:THR:HG21	1:B:357:ARG:HH12	1.70	0.55
1:B:487:ARG:O	1:B:491:THR:HG23	2.06	0.55
1:D:471:MET:HE2	1:D:475:TRP:CH2	2.40	0.55
1:B:443:LYS:HG2	1:B:448:GLN:NE2	2.17	0.55
1:D:389:ASN:HD21	1:D:391:LYS:HB3	1.72	0.55
1:A:244:ARG:HH11	1:A:244:ARG:HG2	1.71	0.55
1:A:332:ARG:NH2	1:A:369:PRO:CG	2.65	0.55
1:A:390:MET:HE2	1:A:396:PHE:HE2	1.72	0.55
1:D:248:ILE:CD1	1:D:355:ALA:HB3	2.36	0.55
1:E:248:ILE:O	1:E:252:VAL:HG22	2.07	0.55
1:E:294:ARG:HD2	1:E:295:TYR:CZ	2.41	0.55
1:A:362:THR:HG22	1:A:364:THR:HG23	1.88	0.55
1:B:372:ARG:HG3	1:B:372:ARG:O	2.06	0.55
1:D:422:GLU:N	1:D:422:GLU:OE1	2.40	0.55
1:A:428:TYR:CD1	1:A:441:MET:HE1	2.42	0.55
1:C:204:THR:HG22	1:C:224:TRP:HE1	1.70	0.55
1:C:390:MET:HE2	1:C:396:PHE:HE2	1.71	0.55
1:D:204:THR:HG22	1:D:224:TRP:HE1	1.71	0.55
1:A:204:THR:HG22	1:A:224:TRP:HE1	1.71	0.55
1:C:240:ARG:O	1:C:244:ARG:HB2	2.07	0.55
1:D:424:TYR:OH	1:D:426:LEU:HD23	2.07	0.55
1:D:466:VAL:O	1:D:469:LYS:HB3	2.07	0.55
1:E:186:THR:HG22	1:E:187:SER:N	2.22	0.55
1:C:487:ARG:O	1:C:491:THR:HG23	2.07	0.54
1:E:389:ASN:HD21	1:E:391:LYS:HB3	1.72	0.54
1:A:435:ASP:N	1:A:436:PRO:HD3	2.22	0.54
1:C:294:ARG:HD2	1:C:295:TYR:CZ	2.42	0.54
1:D:198:GLN:HE22	1:D:250:GLN:NE2	2.05	0.54
1:D:244:ARG:HG2	1:D:244:ARG:HH11	1.72	0.54
1:B:248:ILE:HD13	1:B:355:ALA:HB3	1.89	0.54
1:A:331:HIS:HD2	1:A:333:ASP:H	1.54	0.54
1:C:198:GLN:HE22	1:C:250:GLN:NE2	2.04	0.54
1:C:413:ARG:NH1	1:C:423:ASP:O	2.40	0.54
1:D:428:TYR:CD1	1:D:441:MET:HE1	2.42	0.54
1:D:462:GLU:O	1:D:466:VAL:HG23	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:413:ARG:NH1	1:E:423:ASP:O	2.40	0.54
1:A:198:GLN:HE22	1:A:250:GLN:NE2	2.06	0.54
1:A:471:MET:HE2	1:A:475:TRP:CH2	2.43	0.54
1:E:213:LYS:HG2	1:E:218:GLU:HG2	1.88	0.54
1:B:184:MET:HE3	1:B:192:GLY:HA2	1.88	0.54
1:C:488:ILE:O	1:C:492:LEU:HB2	2.08	0.54
1:A:424:TYR:OH	1:A:426:LEU:HD23	2.07	0.54
1:C:244:ARG:HH22	1:C:366:ASP:HB3	1.71	0.54
1:D:362:THR:HG22	1:D:362:THR:O	2.08	0.54
1:D:362:THR:HG22	1:D:364:THR:HG23	1.89	0.54
1:D:365:ILE:HD11	1:D:393:PHE:CD1	2.42	0.54
1:A:330:ALA:HB3	1:A:356:VAL:CG2	2.38	0.54
1:B:428:TYR:CD1	1:B:441:MET:HE1	2.43	0.53
1:A:213:LYS:HG2	1:A:218:GLU:HG2	1.90	0.53
1:A:248:ILE:HD13	1:A:355:ALA:HB3	1.90	0.53
1:A:330:ALA:HB3	1:A:356:VAL:HG22	1.91	0.53
1:D:390:MET:HE2	1:D:396:PHE:HE2	1.74	0.53
1:B:204:THR:HG22	1:B:224:TRP:HE1	1.70	0.53
1:E:362:THR:HG22	1:E:362:THR:O	2.08	0.53
1:E:443:LYS:HG2	1:E:448:GLN:NE2	2.18	0.53
1:B:330:ALA:HB3	1:B:356:VAL:CG2	2.38	0.53
1:B:389:ASN:HD21	1:B:391:LYS:HB3	1.72	0.53
1:A:326:LYS:NZ	1:A:327:PRO:O	2.42	0.53
1:B:394:GLU:OE2	1:B:397:LYS:HD2	2.09	0.53
1:C:267:ASN:ND2	1:C:267:ASN:N	2.50	0.53
1:B:390:MET:HE2	1:B:396:PHE:HE2	1.74	0.53
1:C:330:ALA:HB3	1:C:356:VAL:HG22	1.91	0.53
1:D:331:HIS:HD2	1:D:333:ASP:H	1.56	0.53
1:A:389:ASN:HD21	1:A:391:LYS:HB3	1.74	0.53
1:A:413:ARG:NH1	1:A:423:ASP:O	2.42	0.53
1:B:413:ARG:NH1	1:B:423:ASP:O	2.42	0.53
1:E:376:LYS:HA	1:E:379:MET:HG3	1.89	0.53
1:E:390:MET:HE2	1:E:396:PHE:HE2	1.74	0.53
1:B:254:LEU:HD21	1:B:259:ILE:HD12	1.91	0.53
1:D:213:LYS:HG2	1:D:218:GLU:HG2	1.89	0.53
1:D:326:LYS:HG2	1:D:327:PRO:O	2.09	0.53
1:E:204:THR:HG21	1:E:224:TRP:HE1	1.71	0.53
1:E:240:ARG:O	1:E:244:ARG:HB2	2.09	0.53
1:C:372:ARG:CZ	1:C:438:VAL:HG11	2.39	0.52
1:D:369:PRO:O	1:D:371:HIS:N	2.43	0.52
1:C:204:THR:HG21	1:C:224:TRP:HE1	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:285:HIS:HB2	1:E:341:VAL:O	2.10	0.52
1:C:424:TYR:OH	1:C:426:LEU:HD23	2.10	0.52
1:E:487:ARG:O	1:E:491:THR:HG23	2.08	0.52
1:D:413:ARG:NH1	1:D:423:ASP:O	2.43	0.52
1:A:466:VAL:O	1:A:469:LYS:HB3	2.08	0.52
1:C:323:THR:C	1:C:325:GLY:H	2.17	0.52
1:A:294:ARG:HD2	1:A:295:TYR:CZ	2.44	0.52
1:B:435:ASP:N	1:B:436:PRO:HD3	2.24	0.52
1:C:435:ASP:N	1:C:436:PRO:HD3	2.24	0.52
1:A:413:ARG:NH1	1:A:422:GLU:HB3	2.25	0.52
1:C:299:VAL:O	1:C:303:ILE:HG13	2.10	0.52
1:D:285:HIS:HB2	1:D:341:VAL:O	2.10	0.52
1:D:369:PRO:C	1:D:371:HIS:H	2.18	0.52
1:D:413:ARG:NH1	1:D:422:GLU:HB3	2.25	0.52
1:C:199:ARG:HD3	1:C:266:ASP:OD2	2.10	0.52
1:C:362:THR:HG22	1:C:362:THR:O	2.10	0.52
1:D:240:ARG:O	1:D:244:ARG:HB2	2.10	0.52
1:D:435:ASP:N	1:D:436:PRO:HD3	2.25	0.52
1:C:213:LYS:HG2	1:C:218:GLU:HG2	1.92	0.51
1:C:330:ALA:HB3	1:C:356:VAL:CG2	2.40	0.51
1:A:488:ILE:O	1:A:492:LEU:HB2	2.10	0.51
1:C:267:ASN:HD22	1:C:267:ASN:N	1.91	0.51
1:D:330:ALA:HB3	1:D:356:VAL:HG22	1.93	0.51
1:D:330:ALA:HB3	1:D:356:VAL:CG2	2.40	0.51
1:E:413:ARG:NH1	1:E:422:GLU:HB3	2.26	0.51
1:C:462:GLU:O	1:C:466:VAL:HG23	2.09	0.51
1:E:424:TYR:OH	1:E:426:LEU:HD23	2.10	0.51
1:A:443:LYS:HG2	1:A:448:GLN:NE2	2.17	0.51
1:B:213:LYS:HG2	1:B:218:GLU:HG2	1.92	0.51
1:E:435:ASP:N	1:E:436:PRO:HD3	2.25	0.51
1:D:357:ARG:H	1:D:366:ASP:HB3	1.76	0.51
1:E:330:ALA:HB3	1:E:356:VAL:HG22	1.93	0.51
1:A:298:THR:HG22	1:A:299:VAL:N	2.26	0.51
1:A:462:GLU:O	1:A:466:VAL:HG23	2.11	0.51
1:A:487:ARG:O	1:A:491:THR:HG23	2.10	0.51
1:B:240:ARG:O	1:B:244:ARG:HB2	2.11	0.51
1:B:471:MET:HE2	1:B:475:TRP:CH2	2.46	0.51
1:D:367:ILE:HG13	1:D:369:PRO:HD3	1.91	0.51
1:B:466:VAL:O	1:B:469:LYS:HB3	2.11	0.50
1:D:189:SER:C	1:D:191:SER:H	2.19	0.50
1:D:487:ARG:O	1:D:491:THR:HG23	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:413:ARG:HG2	1:E:422:GLU:HB2	1.92	0.50
1:B:362:THR:HG22	1:B:362:THR:O	2.10	0.50
1:D:204:THR:HG21	1:D:224:TRP:HE1	1.75	0.50
1:B:244:ARG:HG2	1:B:244:ARG:NH1	2.27	0.50
1:C:244:ARG:HH11	1:C:244:ARG:HG2	1.75	0.50
1:C:471:MET:HE2	1:C:475:TRP:CH2	2.47	0.50
1:D:372:ARG:CD	1:D:379:MET:HE1	2.40	0.50
1:D:309:THR:HG22	1:D:404:MET:CE	2.32	0.50
1:D:443:LYS:HG2	1:D:448:GLN:NE2	2.20	0.50
1:A:323:THR:O	1:A:325:GLY:N	2.42	0.50
1:C:356:VAL:HG23	1:C:393:PHE:HE1	1.76	0.50
1:C:413:ARG:NH1	1:C:422:GLU:HB3	2.27	0.50
1:D:488:ILE:O	1:D:492:LEU:HB2	2.11	0.50
1:B:251:THR:HG22	1:B:252:VAL:HG23	1.94	0.50
1:E:298:THR:HG22	1:E:299:VAL:N	2.25	0.50
1:E:462:GLU:O	1:E:466:VAL:HG23	2.11	0.50
1:A:184:MET:HE3	1:A:192:GLY:HA2	1.92	0.50
1:B:413:ARG:NH1	1:B:422:GLU:HB3	2.26	0.50
1:D:246:ALA:HB2	1:D:278:LEU:HD11	1.92	0.50
1:E:488:ILE:O	1:E:492:LEU:HB2	2.12	0.50
1:A:184:MET:CE	1:A:255:ARG:NH1	2.73	0.49
1:B:413:ARG:HG2	1:B:422:GLU:HB2	1.94	0.49
1:C:298:THR:HG22	1:C:299:VAL:N	2.27	0.49
1:B:298:THR:HG22	1:B:299:VAL:N	2.27	0.49
1:B:331:HIS:HD2	1:B:333:ASP:N	2.10	0.49
1:C:319:GLU:OE1	1:C:360:SER:HB3	2.12	0.49
1:C:332:ARG:HH21	1:C:367:ILE:HD12	1.77	0.49
1:E:224:TRP:CH2	1:E:225:ARG:HD2	2.48	0.49
1:D:369:PRO:HB2	1:D:390:MET:SD	2.53	0.49
1:A:190:GLY:O	1:A:253:MET:HB2	2.12	0.49
1:A:362:THR:HG22	1:A:362:THR:O	2.13	0.49
1:A:413:ARG:HG2	1:A:422:GLU:HB2	1.93	0.49
1:C:331:HIS:HD2	1:C:333:ASP:N	2.10	0.49
1:E:244:ARG:HG2	1:E:244:ARG:NH1	2.25	0.49
1:C:494:GLN:O	1:C:497:GLN:HB3	2.13	0.49
1:D:299:VAL:O	1:D:303:ILE:HG13	2.12	0.49
1:E:205:ILE:CG2	1:E:206:VAL:N	2.76	0.49
1:A:184:MET:HE2	1:A:255:ARG:HH12	1.72	0.49
1:A:248:ILE:O	1:A:252:VAL:HG22	2.13	0.49
1:C:285:HIS:HB3	1:C:341:VAL:HG13	1.95	0.49
1:E:466:VAL:O	1:E:469:LYS:HB3	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:184:MET:CE	1:A:255:ARG:HH12	2.25	0.49
1:A:215:ARG:HH12	1:A:374:GLY:HA2	1.77	0.49
1:E:331:HIS:HD2	1:E:333:ASP:N	2.11	0.49
1:B:300:GLU:HG3	1:B:501:ILE:HG12	1.93	0.48
1:E:330:ALA:HB3	1:E:356:VAL:CG2	2.44	0.48
1:B:285:HIS:HB2	1:B:341:VAL:O	2.13	0.48
1:A:199:ARG:HD3	1:A:266:ASP:OD2	2.13	0.48
1:D:413:ARG:HG2	1:D:422:GLU:HB2	1.95	0.48
1:E:394:GLU:OE2	1:E:397:LYS:HD2	2.13	0.48
1:B:488:ILE:O	1:B:492:LEU:HB2	2.13	0.48
1:C:443:LYS:HG2	1:C:448:GLN:NE2	2.21	0.48
1:D:298:THR:HG22	1:D:299:VAL:N	2.28	0.48
1:E:342:LYS:HA	2:E:1:SO4:O4	2.13	0.48
1:E:346:THR:HG22	1:E:347:CYS:H	1.78	0.48
1:B:204:THR:HG21	1:B:224:TRP:HE1	1.76	0.48
1:C:303:ILE:HG21	1:C:496:SER:HB2	1.95	0.48
1:D:467:MET:O	1:D:471:MET:HG3	2.14	0.48
1:A:425:GLN:HB3	1:A:429:TYR:CD2	2.49	0.48
1:D:394:GLU:OE2	1:D:397:LYS:HD2	2.13	0.48
1:E:471:MET:HE2	1:E:475:TRP:CH2	2.48	0.48
1:A:244:ARG:HG2	1:A:244:ARG:NH1	2.29	0.48
1:C:303:ILE:CG2	1:C:496:SER:HB2	2.43	0.48
1:B:425:GLN:HB3	1:B:429:TYR:CD2	2.48	0.48
1:C:409:TRP:CB	1:C:471:MET:HE3	2.41	0.48
1:C:394:GLU:OE2	1:C:397:LYS:HD2	2.14	0.47
1:C:413:ARG:HG2	1:C:422:GLU:HB2	1.96	0.47
1:C:442:ARG:O	1:C:446:CYS:HB2	2.14	0.47
1:E:457:ARG:C	1:E:459:GLN:H	2.21	0.47
1:A:251:THR:HG21	1:A:357:ARG:HH12	1.79	0.47
1:C:457:ARG:C	1:C:459:GLN:H	2.22	0.47
1:E:489:LYS:O	1:E:493:SER:HB2	2.15	0.47
1:D:248:ILE:O	1:D:252:VAL:HB	2.15	0.47
1:E:442:ARG:O	1:E:446:CYS:HB2	2.14	0.47
1:C:253:MET:O	1:C:254:LEU:C	2.57	0.47
1:A:323:THR:C	1:A:325:GLY:N	2.73	0.47
1:A:356:VAL:HG23	1:A:393:PHE:HE1	1.79	0.47
1:A:365:ILE:HD12	1:A:365:ILE:H	1.78	0.47
1:B:198:GLN:HB3	1:B:264:ALA:HB1	1.97	0.47
1:C:183:ASP:O	1:C:187:SER:HB2	2.15	0.47
1:C:425:GLN:HB3	1:C:429:TYR:CD2	2.50	0.47
1:D:204:THR:HG22	1:D:224:TRP:NE1	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:308:SER:OG	1:D:347:CYS:HB2	2.15	0.47
1:D:372:ARG:CG	1:D:379:MET:HE1	2.43	0.47
1:D:442:ARG:O	1:D:446:CYS:HB2	2.14	0.47
1:D:457:ARG:C	1:D:459:GLN:H	2.23	0.47
1:B:424:TYR:OH	1:B:426:LEU:HD23	2.14	0.47
1:D:224:TRP:CH2	1:D:225:ARG:HD2	2.50	0.47
1:A:394:GLU:OE2	1:A:397:LYS:HD2	2.15	0.47
1:B:254:LEU:C	1:B:254:LEU:CD2	2.88	0.47
1:A:346:THR:HG22	1:A:347:CYS:H	1.80	0.47
1:B:344:ASN:CG	1:B:346:THR:HG1	2.23	0.47
1:E:234:PHE:CE1	1:E:278:LEU:HD22	2.50	0.47
1:E:467:MET:O	1:E:471:MET:HG3	2.15	0.47
1:B:252:VAL:C	1:B:253:MET:HG3	2.40	0.46
1:D:244:ARG:HG2	1:D:244:ARG:NH1	2.30	0.46
1:E:242:TRP:CD1	1:E:278:LEU:HD13	2.51	0.46
1:E:365:ILE:HG22	1:E:367:ILE:HG23	1.97	0.46
1:E:468:ALA:O	1:E:472:ARG:HG3	2.16	0.46
1:C:199:ARG:HD2	1:C:203:ARG:NE	2.29	0.46
1:C:365:ILE:CG2	1:C:366:ASP:N	2.78	0.46
1:D:249:TYR:CD2	1:D:262:PHE:HB2	2.50	0.46
1:A:299:VAL:O	1:A:303:ILE:HG13	2.15	0.46
1:B:442:ARG:O	1:B:446:CYS:HB2	2.15	0.46
1:A:459:GLN:NE2	1:A:465:ARG:CG	2.79	0.46
1:A:469:LYS:O	1:A:473:GLU:HG3	2.16	0.46
1:B:457:ARG:C	1:B:459:GLN:H	2.23	0.46
1:D:205:ILE:CG2	1:D:206:VAL:N	2.78	0.46
1:E:229:VAL:HG22	1:E:280:SER:O	2.16	0.46
1:A:459:GLN:HE22	1:A:465:ARG:HG2	1.81	0.46
1:B:204:THR:HG22	1:B:224:TRP:NE1	2.31	0.46
1:C:466:VAL:O	1:C:469:LYS:HB3	2.16	0.46
1:D:372:ARG:HD3	1:D:379:MET:CE	2.43	0.46
1:E:248:ILE:CD1	1:E:355:ALA:HB3	2.45	0.46
1:A:297:VAL:CG2	1:A:298:THR:N	2.79	0.46
1:E:190:GLY:O	1:E:191:SER:C	2.59	0.46
1:E:299:VAL:O	1:E:303:ILE:HG13	2.14	0.46
1:E:367:ILE:CG1	1:E:370:ASN:HD21	2.26	0.46
1:A:240:ARG:O	1:A:244:ARG:HB2	2.16	0.46
1:B:299:VAL:O	1:B:303:ILE:HG13	2.16	0.46
1:D:372:ARG:HG2	1:D:379:MET:CE	2.45	0.46
1:E:497:GLN:O	1:E:497:GLN:HG2	2.15	0.46
1:B:270:ASN:O	1:B:271:GLY:C	2.58	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:252:VAL:O	1:C:253:MET:CB	2.60	0.46
1:D:285:HIS:HB3	1:D:341:VAL:HG13	1.98	0.46
1:E:367:ILE:HG12	1:E:370:ASN:ND2	2.29	0.46
1:B:224:TRP:CH2	1:B:225:ARG:HD2	2.50	0.46
1:B:298:THR:CG2	1:B:299:VAL:N	2.79	0.46
1:B:420:ILE:HG13	1:B:420:ILE:O	2.16	0.46
1:C:492:LEU:HD12	1:C:492:LEU:HA	1.84	0.46
1:D:253:MET:CE	1:D:324:GLN:HA	2.46	0.46
1:D:425:GLN:HB3	1:D:429:TYR:CD2	2.50	0.46
1:E:367:ILE:HD12	1:E:367:ILE:H	1.81	0.46
1:C:346:THR:HG22	1:C:347:CYS:H	1.80	0.46
1:C:385:ASP:OD1	1:C:387:SER:N	2.49	0.46
1:E:171:ILE:HD12	1:E:200:THR:CG2	2.46	0.46
1:E:187:SER:O	1:E:188:GLY:C	2.59	0.46
1:A:234:PHE:CE1	1:A:278:LEU:HD22	2.51	0.45
1:A:298:THR:CG2	1:A:299:VAL:N	2.79	0.45
1:A:331:HIS:HD2	1:A:333:ASP:N	2.12	0.45
1:A:343:LYS:HB2	2:A:9:SO4:O3	2.17	0.45
1:A:467:MET:O	1:A:471:MET:HG3	2.15	0.45
1:B:247:GLU:O	1:B:251:THR:HB	2.16	0.45
1:C:297:VAL:CG2	1:C:298:THR:N	2.79	0.45
1:C:489:LYS:O	1:C:493:SER:HB2	2.16	0.45
1:D:365:ILE:HG23	1:D:366:ASP:N	2.30	0.45
1:E:298:THR:CG2	1:E:299:VAL:N	2.78	0.45
1:C:469:LYS:O	1:C:473:GLU:HG3	2.16	0.45
1:A:248:ILE:CD1	1:A:355:ALA:HB3	2.47	0.45
1:A:459:GLN:NE2	1:A:459:GLN:HA	2.31	0.45
1:C:357:ARG:HB2	1:C:366:ASP:CG	2.42	0.45
1:D:469:LYS:O	1:D:473:GLU:HG3	2.16	0.45
1:D:489:LYS:O	1:D:493:SER:HB2	2.16	0.45
1:E:469:LYS:O	1:E:473:GLU:HG3	2.16	0.45
1:B:205:ILE:CG2	1:B:206:VAL:N	2.80	0.45
1:B:240:ARG:NH1	1:B:240:ARG:HB2	2.32	0.45
1:C:199:ARG:NH1	1:C:203:ARG:NH2	2.64	0.45
1:E:432:VAL:HA	1:E:433:PRO:HD3	1.81	0.45
1:A:190:GLY:HA3	1:A:253:MET:HE3	1.97	0.45
1:C:205:ILE:CG2	1:C:206:VAL:N	2.79	0.45
1:C:420:ILE:HG13	1:C:420:ILE:O	2.15	0.45
1:D:294:ARG:O	1:D:294:ARG:HD3	2.17	0.45
1:D:346:THR:HG22	1:D:347:CYS:H	1.81	0.45
1:E:199:ARG:NH1	1:E:203:ARG:NH2	2.65	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:346:THR:HG22	1:B:347:CYS:H	1.81	0.45
1:D:297:VAL:CG2	1:D:298:THR:N	2.80	0.45
1:E:190:GLY:O	1:E:192:GLY:N	2.49	0.45
1:A:442:ARG:O	1:A:446:CYS:HB2	2.16	0.45
1:B:195:LEU:HD12	1:B:195:LEU:N	2.32	0.45
1:B:215:ARG:HH11	1:B:354:LEU:HD11	1.81	0.45
1:B:297:VAL:CG2	1:B:298:THR:N	2.79	0.45
1:B:356:VAL:HG23	1:B:393:PHE:HE1	1.82	0.45
1:B:447:GLU:C	1:B:449:LYS:H	2.25	0.45
1:C:184:MET:HE3	1:C:192:GLY:HA2	1.98	0.45
1:C:459:GLN:HE22	1:C:465:ARG:HG2	1.82	0.45
1:D:199:ARG:NH1	1:D:203:ARG:NH2	2.65	0.45
1:E:409:TRP:CB	1:E:471:MET:HE3	2.43	0.45
1:D:199:ARG:HD2	1:D:203:ARG:NE	2.32	0.45
1:D:492:LEU:HD12	1:D:492:LEU:HA	1.85	0.45
1:A:205:ILE:CG2	1:A:206:VAL:N	2.79	0.45
1:C:294:ARG:O	1:C:294:ARG:HD3	2.17	0.45
1:D:171:ILE:HD11	1:D:197:VAL:HG13	1.98	0.45
1:A:420:ILE:HG13	1:A:420:ILE:O	2.16	0.44
1:C:229:VAL:HG22	1:C:280:SER:O	2.16	0.44
1:D:358:HIS:HB2	1:D:393:PHE:CD1	2.51	0.44
1:D:368:ALA:C	1:D:370:ASN:N	2.75	0.44
1:D:409:TRP:CB	1:D:471:MET:HE3	2.44	0.44
1:D:458:TRP:CG	1:D:464:LEU:HD12	2.52	0.44
1:A:457:ARG:C	1:A:459:GLN:H	2.24	0.44
1:C:244:ARG:HG2	1:C:244:ARG:NH1	2.32	0.44
1:E:420:ILE:O	1:E:420:ILE:HG13	2.16	0.44
1:A:224:TRP:CH2	1:A:225:ARG:HD2	2.53	0.44
1:B:409:TRP:CB	1:B:471:MET:HE3	2.42	0.44
1:B:432:VAL:HA	1:B:433:PRO:HD3	1.83	0.44
1:C:498:GLN:O	1:C:499:GLU:CG	2.64	0.44
1:D:195:LEU:N	1:D:195:LEU:HD12	2.31	0.44
1:D:344:ASN:CG	1:D:346:THR:HG1	2.26	0.44
1:D:459:GLN:HA	1:D:459:GLN:NE2	2.33	0.44
1:E:297:VAL:CG2	1:E:298:THR:N	2.80	0.44
1:A:371:HIS:O	1:A:373:VAL:HG13	2.18	0.44
1:C:204:THR:HG22	1:C:224:TRP:NE1	2.31	0.44
1:C:298:THR:CG2	1:C:299:VAL:N	2.79	0.44
1:C:365:ILE:CG2	1:C:366:ASP:H	2.30	0.44
1:E:308:SER:OG	1:E:347:CYS:HB2	2.16	0.44
1:E:331:HIS:O	1:E:332:ARG:HB2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:425:GLN:HB3	1:E:429:TYR:CD2	2.52	0.44
1:A:468:ALA:O	1:A:472:ARG:HG3	2.18	0.44
1:A:489:LYS:O	1:A:493:SER:HB2	2.18	0.44
1:B:215:ARG:NH1	1:B:354:LEU:HD11	2.32	0.44
1:B:458:TRP:CG	1:B:464:LEU:HD12	2.52	0.44
1:E:294:ARG:HD3	1:E:294:ARG:O	2.18	0.44
1:A:285:HIS:HB2	1:A:341:VAL:O	2.17	0.44
1:A:294:ARG:O	1:A:294:ARG:HD3	2.17	0.44
1:B:199:ARG:HD2	1:B:203:ARG:NE	2.33	0.44
1:C:447:GLU:C	1:C:449:LYS:H	2.25	0.44
1:D:298:THR:CG2	1:D:299:VAL:N	2.81	0.44
1:E:428:TYR:O	1:E:432:VAL:HG12	2.18	0.44
1:A:458:TRP:CG	1:A:464:LEU:HD12	2.53	0.44
1:B:462:GLU:O	1:B:466:VAL:HG23	2.17	0.44
1:C:459:GLN:NE2	1:C:465:ARG:CG	2.81	0.44
1:D:420:ILE:HG13	1:D:420:ILE:O	2.16	0.44
1:A:270:ASN:O	1:A:271:GLY:C	2.61	0.44
1:C:287:SER:HA	1:C:340:LEU:HD23	2.00	0.44
1:D:317:HIS:HD2	1:D:329:ILE:O	2.01	0.44
1:E:270:ASN:O	1:E:271:GLY:C	2.60	0.43
1:E:458:TRP:CG	1:E:464:LEU:HD12	2.52	0.43
1:C:270:ASN:O	1:C:271:GLY:C	2.60	0.43
1:E:199:ARG:HD2	1:E:203:ARG:NE	2.32	0.43
1:E:205:ILE:HG22	1:E:206:VAL:N	2.33	0.43
1:A:366:ASP:O	1:A:366:ASP:OD2	2.36	0.43
1:A:454:ILE:HG23	1:A:458:TRP:CE3	2.54	0.43
1:B:459:GLN:HA	1:B:459:GLN:NE2	2.34	0.43
1:E:253:MET:O	1:E:254:LEU:C	2.61	0.43
1:A:240:ARG:HB2	1:A:240:ARG:NH1	2.34	0.43
1:D:331:HIS:HD2	1:D:333:ASP:N	2.16	0.43
1:A:195:LEU:N	1:A:195:LEU:HD12	2.33	0.43
1:B:489:LYS:O	1:B:493:SER:HB2	2.18	0.43
1:C:306:ALA:HB1	1:C:492:LEU:HD21	2.00	0.43
1:C:467:MET:O	1:C:471:MET:HG3	2.17	0.43
1:D:459:GLN:HE22	1:D:465:ARG:HG2	1.84	0.43
1:A:199:ARG:NH1	1:A:203:ARG:NH2	2.66	0.43
1:A:323:THR:OG1	1:A:324:GLN:N	2.50	0.43
1:B:428:TYR:O	1:B:432:VAL:HG12	2.18	0.43
1:C:291:TYR:CG	1:C:341:VAL:HG11	2.52	0.43
1:D:447:GLU:C	1:D:449:LYS:H	2.26	0.43
1:A:204:THR:HG21	1:A:224:TRP:HE1	1.78	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:414:ARG:HD2	1:D:424:TYR:HB2	2.01	0.43
1:B:211:ILE:O	1:B:211:ILE:HG22	2.19	0.43
1:B:331:HIS:CD2	1:B:333:ASP:H	2.34	0.43
1:B:362:THR:HG22	1:B:364:THR:CG2	2.49	0.43
1:C:458:TRP:CG	1:C:464:LEU:HD12	2.53	0.43
1:C:459:GLN:NE2	1:C:459:GLN:HA	2.34	0.43
1:D:237:ARG:O	1:D:237:ARG:HG2	2.19	0.43
1:E:195:LEU:HD12	1:E:195:LEU:N	2.33	0.43
1:E:459:GLN:HA	1:E:459:GLN:NE2	2.34	0.43
1:A:428:TYR:O	1:A:432:VAL:HG12	2.19	0.43
1:D:211:ILE:O	1:D:211:ILE:HG22	2.17	0.43
1:A:204:THR:HG22	1:A:224:TRP:NE1	2.32	0.43
1:A:447:GLU:C	1:A:449:LYS:H	2.26	0.43
1:C:190:GLY:CA	1:C:324:GLN:HE22	2.27	0.43
1:C:428:TYR:O	1:C:432:VAL:HG12	2.19	0.43
1:B:307:LEU:HA	1:B:492:LEU:HD23	2.01	0.42
1:C:297:VAL:CG2	1:C:301:GLY:HA3	2.48	0.42
1:E:365:ILE:N	1:E:365:ILE:HD12	2.34	0.42
1:C:195:LEU:HD12	1:C:195:LEU:N	2.34	0.42
1:C:371:HIS:CG	1:C:372:ARG:N	2.80	0.42
1:C:428:TYR:HD1	1:C:441:MET:HE1	1.83	0.42
1:A:372:ARG:CG	1:A:379:MET:CE	2.94	0.42
1:C:473:GLU:HB2	1:C:483:LEU:CD1	2.49	0.42
1:D:468:ALA:O	1:D:472:ARG:HG3	2.19	0.42
1:E:362:THR:HG22	1:E:364:THR:CG2	2.50	0.42
1:E:390:MET:HE2	1:E:396:PHE:CE2	2.54	0.42
1:A:344:ASN:CG	1:A:346:THR:HG1	2.27	0.42
1:A:470:ILE:HD13	1:A:488:ILE:HG23	2.01	0.42
1:B:495:LEU:O	1:B:499:GLU:HG2	2.19	0.42
1:C:368:ALA:CB	1:C:369:PRO:CD	2.95	0.42
1:C:372:ARG:HD2	1:C:383:VAL:O	2.19	0.42
1:C:433:PRO:O	1:C:436:PRO:HG3	2.19	0.42
1:D:253:MET:HE1	1:D:324:GLN:HA	2.01	0.42
1:A:390:MET:HE2	1:A:396:PHE:CE2	2.53	0.42
1:B:385:ASP:OD1	1:B:387:SER:N	2.51	0.42
1:D:252:VAL:O	1:D:253:MET:CG	2.58	0.42
1:D:459:GLN:NE2	1:D:465:ARG:CG	2.82	0.42
1:E:204:THR:HG22	1:E:224:TRP:NE1	2.28	0.42
1:B:294:ARG:O	1:B:294:ARG:HD3	2.20	0.42
1:B:433:PRO:O	1:B:436:PRO:HG3	2.19	0.42
1:C:490:LYS:HE3	1:C:490:LYS:HB2	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:270:ASN:O	1:D:271:GLY:C	2.63	0.42
1:E:428:TYR:HD1	1:E:441:MET:HE1	1.84	0.42
1:A:409:TRP:CB	1:A:471:MET:HE3	2.45	0.42
1:C:432:VAL:HA	1:C:433:PRO:HD3	1.82	0.42
1:D:447:GLU:C	1:D:449:LYS:N	2.78	0.42
1:A:251:THR:HG21	1:A:357:ARG:NH1	2.34	0.42
1:B:308:SER:HB2	1:B:346:THR:HG22	2.02	0.42
1:B:467:MET:O	1:B:471:MET:HG3	2.19	0.42
1:D:242:TRP:CD1	1:D:278:LEU:HD13	2.54	0.42
1:D:368:ALA:O	1:D:370:ASN:N	2.52	0.42
1:D:432:VAL:HA	1:D:433:PRO:HD3	1.80	0.42
1:B:447:GLU:C	1:B:449:LYS:N	2.78	0.42
1:B:490:LYS:HE3	1:B:490:LYS:HB2	1.86	0.42
1:D:470:ILE:HD13	1:D:488:ILE:HG23	2.01	0.42
1:E:211:ILE:O	1:E:211:ILE:HG22	2.18	0.42
1:A:197:VAL:O	1:A:201:ILE:HG13	2.20	0.41
1:B:390:MET:HE2	1:B:396:PHE:CE2	2.53	0.41
1:C:390:MET:HE2	1:C:396:PHE:CE2	2.52	0.41
1:C:457:ARG:O	1:C:460:SER:OG	2.35	0.41
1:C:470:ILE:HD13	1:C:488:ILE:HG23	2.02	0.41
1:D:357:ARG:H	1:D:366:ASP:CB	2.33	0.41
1:E:367:ILE:HG21	1:E:370:ASN:OD1	2.20	0.41
1:C:193:LEU:HA	1:C:194:PRO:HD3	1.93	0.41
1:D:240:ARG:NH1	1:D:240:ARG:HB2	2.35	0.41
1:B:184:MET:O	1:B:188:GLY:HA3	2.20	0.41
1:B:434:SER:O	1:B:435:ASP:HB3	2.21	0.41
1:B:469:LYS:O	1:B:473:GLU:HG3	2.19	0.41
1:C:443:LYS:O	1:C:447:GLU:HB2	2.19	0.41
1:D:229:VAL:HG22	1:D:280:SER:O	2.21	0.41
1:D:331:HIS:O	1:D:332:ARG:HB2	2.19	0.41
1:E:368:ALA:CB	1:E:369:PRO:CD	2.75	0.41
1:C:246:ALA:HB2	1:C:278:LEU:HD11	2.02	0.41
1:C:468:ALA:O	1:C:472:ARG:HG3	2.21	0.41
1:D:252:VAL:CG1	1:D:326:LYS:HB2	2.41	0.41
1:E:358:HIS:HB2	1:E:393:PHE:CD1	2.55	0.41
1:A:183:ASP:O	1:A:187:SER:HB2	2.21	0.41
1:A:443:LYS:O	1:A:447:GLU:HB2	2.20	0.41
1:D:443:LYS:O	1:D:447:GLU:HB2	2.21	0.41
1:E:184:MET:HE3	1:E:192:GLY:HA3	2.02	0.41
1:E:285:HIS:HB3	1:E:341:VAL:HG13	2.02	0.41
1:B:193:LEU:HA	1:B:194:PRO:HD3	1.90	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:343:LYS:HB2	2:B:6:SO4:O4	2.20	0.41
1:E:237:ARG:O	1:E:237:ARG:HG2	2.19	0.41
1:A:492:LEU:HD12	1:A:492:LEU:HA	1.87	0.41
1:D:326:LYS:CB	1:D:327:PRO:HD2	2.51	0.41
1:E:278:LEU:HD12	1:E:278:LEU:HA	1.95	0.41
1:E:331:HIS:CD2	1:E:333:ASP:H	2.35	0.41
1:A:447:GLU:C	1:A:449:LYS:N	2.79	0.41
1:B:358:HIS:HB2	1:B:393:PHE:CD1	2.55	0.41
1:B:428:TYR:HD1	1:B:441:MET:HE1	1.86	0.41
1:E:444:VAL:HG13	1:E:450:LEU:HD12	2.03	0.41
1:A:292:LEU:HD12	1:A:292:LEU:HA	1.90	0.41
1:A:331:HIS:O	1:A:332:ARG:HB2	2.21	0.41
1:A:414:ARG:HD2	1:A:424:TYR:HB2	2.03	0.41
1:A:490:LYS:HE3	1:A:490:LYS:HB2	1.87	0.41
1:B:237:ARG:HG2	1:B:237:ARG:O	2.21	0.41
1:B:331:HIS:O	1:B:332:ARG:HB2	2.21	0.41
1:B:443:LYS:O	1:B:447:GLU:HB2	2.21	0.41
1:B:459:GLN:NE2	1:B:465:ARG:CG	2.83	0.41
1:D:205:ILE:HG22	1:D:206:VAL:N	2.35	0.41
1:D:432:VAL:CG2	1:D:433:PRO:HD2	2.51	0.41
1:E:331:HIS:HE1	1:E:350:ALA:O	2.04	0.41
1:E:414:ARG:HD2	1:E:424:TYR:HB2	2.03	0.41
1:D:433:PRO:O	1:D:436:PRO:HG3	2.21	0.41
1:E:240:ARG:NH1	1:E:240:ARG:HB2	2.36	0.41
1:A:407:VAL:O	1:A:411:ILE:HG13	2.22	0.40
1:B:302:MET:HG3	1:B:411:ILE:HG22	2.02	0.40
1:B:308:SER:OG	1:B:347:CYS:HB2	2.21	0.40
1:B:473:GLU:HB2	1:B:483:LEU:CD1	2.52	0.40
1:C:190:GLY:HA3	1:C:324:GLN:NE2	2.31	0.40
1:C:258:ASN:O	1:C:348:CYS:HA	2.20	0.40
1:C:362:THR:HG22	1:C:364:THR:CG2	2.50	0.40
1:D:376:LYS:N	1:D:376:LYS:HD2	2.36	0.40
1:B:414:ARG:HD2	1:B:424:TYR:HB2	2.03	0.40
1:C:224:TRP:CH2	1:C:225:ARG:HD2	2.57	0.40
1:A:433:PRO:O	1:A:436:PRO:HG3	2.22	0.40
1:A:365:ILE:N	1:A:365:ILE:CD1	2.80	0.40
1:B:459:GLN:HE22	1:B:465:ARG:HG2	1.86	0.40
1:C:237:ARG:HG2	1:C:237:ARG:O	2.21	0.40
1:E:259:ILE:O	1:E:260:LEU:C	2.64	0.40
1:E:323:THR:C	1:E:325:GLY:H	2.29	0.40
1:C:331:HIS:O	1:C:332:ARG:HB2	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:434:SER:O	1:C:435:ASP:HB3	2.21	0.40
1:D:171:ILE:O	1:D:171:ILE:HG22	2.20	0.40
1:E:447:GLU:C	1:E:449:LYS:H	2.29	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:453:ASN:ND2	1:E:453:ASN:ND2[4_566]	2.19	0.01

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	328/342 (96%)	291 (89%)	29 (9%)	8 (2%)	4	18
1	B	318/342 (93%)	284 (89%)	26 (8%)	8 (2%)	4	17
1	C	328/342 (96%)	287 (88%)	33 (10%)	8 (2%)	4	18
1	D	328/342 (96%)	291 (89%)	31 (10%)	6 (2%)	6	25
1	E	328/342 (96%)	291 (89%)	28 (8%)	9 (3%)	4	16
All	All	1630/1710 (95%)	1444 (89%)	147 (9%)	39 (2%)	4	18

All (39) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	369	PRO
1	B	188	GLY
1	D	370	ASN
1	A	323	THR
1	A	324	GLN
1	B	271	GLY

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Mol	Chain	Res	Type
1	C	190	GLY
1	C	254	LEU
1	E	188	GLY
1	E	191	SER
1	A	271	GLY
1	A	447	GLU
1	A	460	SER
1	B	366	ASP
1	B	460	SER
1	C	271	GLY
1	C	460	SER
1	D	460	SER
1	E	271	GLY
1	E	368	ALA
1	E	460	SER
1	B	447	GLU
1	C	447	GLU
1	C	458	TRP
1	D	271	GLY
1	D	447	GLU
1	E	447	GLU
1	B	458	TRP
1	C	448	GLN
1	D	369	PRO
1	D	458	TRP
1	A	448	GLN
1	A	458	TRP
1	B	448	GLN
1	E	458	TRP
1	C	455	PRO
1	E	369	PRO
1	E	455	PRO
1	B	455	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	282/294 (96%)	266 (94%)	16 (6%)	18	49
1	B	278/294 (95%)	261 (94%)	17 (6%)	17	46
1	C	282/294 (96%)	264 (94%)	18 (6%)	16	44
1	D	282/294 (96%)	263 (93%)	19 (7%)	15	43
1	E	282/294 (96%)	263 (93%)	19 (7%)	15	43
All	All	1406/1470 (96%)	1317 (94%)	89 (6%)	16	45

All (89) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	204	THR
1	A	209	GLU
1	A	229	VAL
1	A	244	ARG
1	A	267	ASN
1	A	269	ASP
1	A	278	LEU
1	A	292	LEU
1	A	307	LEU
1	A	326	LYS
1	A	341	VAL
1	A	365	ILE
1	A	367	ILE
1	A	382	GLU
1	A	486	LEU
1	A	491	THR
1	B	204	THR
1	B	209	GLU
1	B	229	VAL
1	B	244	ARG
1	B	251	THR
1	B	254	LEU
1	B	267	ASN
1	B	269	ASP
1	B	278	LEU
1	B	292	LEU
1	B	307	LEU
1	B	326	LYS
1	B	341	VAL
1	B	372	ARG
1	B	382	GLU

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Mol	Chain	Res	Type
1	B	486	LEU
1	B	491	THR
1	C	171	ILE
1	C	204	THR
1	C	209	GLU
1	C	229	VAL
1	C	244	ARG
1	C	253	MET
1	C	255	ARG
1	C	267	ASN
1	C	269	ASP
1	C	278	LEU
1	C	292	LEU
1	C	307	LEU
1	C	341	VAL
1	C	366	ASP
1	C	370	ASN
1	C	382	GLU
1	C	486	LEU
1	C	491	THR
1	D	187	SER
1	D	204	THR
1	D	209	GLU
1	D	229	VAL
1	D	244	ARG
1	D	267	ASN
1	D	269	ASP
1	D	278	LEU
1	D	292	LEU
1	D	307	LEU
1	D	321	VAL
1	D	326	LYS
1	D	341	VAL
1	D	365	ILE
1	D	382	GLU
1	D	486	LEU
1	D	491	THR
1	D	497	GLN
1	D	499	GLU
1	E	204	THR
1	E	209	GLU
1	E	229	VAL

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Mol	Chain	Res	Type
1	E	244	ARG
1	E	267	ASN
1	E	269	ASP
1	E	278	LEU
1	E	292	LEU
1	E	307	LEU
1	E	321	VAL
1	E	323	THR
1	E	326	LYS
1	E	341	VAL
1	E	366	ASP
1	E	367	ILE
1	E	382	GLU
1	E	486	LEU
1	E	491	THR
1	E	499	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (58) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	250	GLN
1	A	256	HIS
1	A	258	ASN
1	A	267	ASN
1	A	275	GLN
1	A	315	HIS
1	A	331	HIS
1	A	389	ASN
1	A	421	HIS
1	A	448	GLN
1	A	459	GLN
1	B	250	GLN
1	B	256	HIS
1	B	258	ASN
1	B	267	ASN
1	B	315	HIS
1	B	331	HIS
1	B	389	ASN
1	B	448	GLN
1	B	459	GLN
1	C	250	GLN
1	C	256	HIS

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Mol	Chain	Res	Type
1	C	258	ASN
1	C	267	ASN
1	C	275	GLN
1	C	315	HIS
1	C	324	GLN
1	C	331	HIS
1	C	389	ASN
1	C	448	GLN
1	C	459	GLN
1	C	497	GLN
1	D	250	GLN
1	D	256	HIS
1	D	258	ASN
1	D	267	ASN
1	D	315	HIS
1	D	331	HIS
1	D	358	HIS
1	D	370	ASN
1	D	371	HIS
1	D	389	ASN
1	D	448	GLN
1	D	459	GLN
1	D	497	GLN
1	E	250	GLN
1	E	256	HIS
1	E	258	ASN
1	E	267	ASN
1	E	275	GLN
1	E	315	HIS
1	E	331	HIS
1	E	358	HIS
1	E	370	ASN
1	E	389	ASN
1	E	421	HIS
1	E	448	GLN
1	E	459	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

15 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	SO4	B	11	-	4,4,4	0.38	0	6,6,6	0.18	0
2	SO4	E	1	-	4,4,4	0.38	0	6,6,6	0.39	0
2	SO4	D	15	-	4,4,4	0.44	0	6,6,6	0.08	0
2	SO4	E	20	-	4,4,4	0.41	0	6,6,6	0.15	0
2	SO4	B	6	-	4,4,4	0.38	0	6,6,6	0.22	0
2	SO4	D	13	-	4,4,4	0.42	0	6,6,6	0.08	0
2	SO4	A	9	-	4,4,4	0.40	0	6,6,6	0.13	0
2	SO4	A	18	-	4,4,4	0.40	0	6,6,6	0.13	0
2	SO4	D	14	-	4,4,4	0.37	0	6,6,6	0.19	0
2	SO4	A	21	-	4,4,4	0.42	0	6,6,6	0.08	0
2	SO4	E	2	-	4,4,4	0.38	0	6,6,6	0.11	0
2	SO4	B	12	-	4,4,4	0.44	0	6,6,6	0.22	0
2	SO4	C	5	-	4,4,4	0.41	0	6,6,6	0.10	0
2	SO4	C	4	-	4,4,4	0.45	0	6,6,6	0.20	0
2	SO4	C	10	-	4,4,4	0.42	0	6,6,6	0.11	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.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	1	SO4	2	0
2	B	6	SO4	1	0
2	A	9	SO4	1	0

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	330/342 (96%)	0.77	28 (8%)	16	14	38, 78, 104, 120	0
1	B	324/342 (94%)	0.55	23 (7%)	22	17	34, 60, 93, 108	0
1	C	330/342 (96%)	1.02	51 (15%)	5	4	34, 77, 103, 124	0
1	D	330/342 (96%)	0.72	36 (10%)	10	9	30, 65, 98, 109	0
1	E	330/342 (96%)	0.57	29 (8%)	15	13	30, 57, 94, 107	0
All	All	1644/1710 (96%)	0.73	167 (10%)	12	10	30, 67, 101, 124	0

All (167) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	367	ILE	5.3
1	B	371	HIS	5.3
1	B	367	ILE	5.2
1	C	450	LEU	5.1
1	A	367	ILE	4.9
1	D	422	GLU	4.7
1	C	481	ALA	4.5
1	E	368	ALA	4.5
1	E	450	LEU	4.5
1	D	500	GLY	4.2
1	C	323	THR	4.1
1	A	487	ARG	4.1
1	C	369	PRO	4.0
1	D	253	MET	4.0
1	C	371	HIS	4.0
1	A	366	ASP	3.9
1	C	476	TYR	3.9
1	C	367	ILE	3.9
1	D	322	GLY	3.8
1	E	456	ASN	3.8

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Mol	Chain	Res	Type	RSRZ
1	D	236	SER	3.8
1	B	251	THR	3.8
1	E	453	ASN	3.7
1	A	369	PRO	3.6
1	D	457	ARG	3.6
1	E	323	THR	3.6
1	C	361	ALA	3.5
1	C	453	ASN	3.5
1	C	426	LEU	3.5
1	C	295	TYR	3.5
1	C	365	ILE	3.4
1	D	325	GLY	3.4
1	B	456	ASN	3.4
1	E	369	PRO	3.4
1	D	363	ASP	3.4
1	C	325	GLY	3.4
1	C	452	PRO	3.4
1	A	253	MET	3.4
1	D	458	TRP	3.3
1	D	417	ILE	3.3
1	C	443	LYS	3.3
1	D	420	ILE	3.3
1	A	490	LYS	3.3
1	C	500	GLY	3.3
1	C	190	GLY	3.2
1	B	214	GLY	3.1
1	D	292	LEU	3.1
1	A	252	VAL	3.1
1	E	432	VAL	3.1
1	D	394	GLU	3.1
1	B	253	MET	3.0
1	B	325	GLY	3.0
1	E	324	GLN	3.0
1	C	472	ARG	3.0
1	C	448	GLN	3.0
1	D	432	VAL	3.0
1	C	479	GLY	3.0
1	A	461	CYS	3.0
1	E	370	ASN	2.9
1	B	186	THR	2.9
1	C	470	ILE	2.9
1	A	325	GLY	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	369	PRO	2.9
1	E	190	GLY	2.8
1	D	423	ASP	2.8
1	D	438	VAL	2.8
1	A	358	HIS	2.8
1	A	417	ILE	2.8
1	E	444	VAL	2.8
1	E	431	LEU	2.8
1	D	480	ALA	2.7
1	C	324	GLN	2.7
1	D	215	ARG	2.7
1	C	439	GLU	2.7
1	C	253	MET	2.7
1	E	188	GLY	2.7
1	A	371	HIS	2.6
1	C	475	TRP	2.6
1	E	500	GLY	2.6
1	E	191	SER	2.6
1	C	487	ARG	2.6
1	A	455	PRO	2.6
1	B	455	PRO	2.6
1	C	368	ALA	2.6
1	D	270	ASN	2.5
1	E	437	SER	2.5
1	B	254	LEU	2.5
1	C	427	PRO	2.5
1	E	254	LEU	2.5
1	C	393	PHE	2.5
1	A	370	ASN	2.5
1	C	358	HIS	2.5
1	A	420	ILE	2.5
1	D	191	SER	2.5
1	D	192	GLY	2.5
1	B	252	VAL	2.5
1	D	390	MET	2.4
1	B	215	ARG	2.4
1	C	186	THR	2.4
1	E	438	VAL	2.4
1	B	440	GLU	2.4
1	C	391	LYS	2.4
1	D	439	GLU	2.4
1	B	361	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	372	ARG	2.4
1	C	457	ARG	2.4
1	D	372	ARG	2.4
1	C	458	TRP	2.4
1	E	366	ASP	2.4
1	C	380	ALA	2.4
1	C	451	ARG	2.3
1	C	183	ASP	2.3
1	C	422	GLU	2.3
1	C	421	HIS	2.3
1	A	321	VAL	2.3
1	D	290	ASP	2.3
1	D	497	GLN	2.3
1	E	371	HIS	2.3
1	A	323	THR	2.3
1	B	391	LYS	2.3
1	A	237	ARG	2.3
1	C	383	VAL	2.3
1	E	321	VAL	2.3
1	E	252	VAL	2.3
1	B	216	PHE	2.3
1	B	319	GLU	2.3
1	C	379	MET	2.3
1	E	391	LYS	2.3
1	A	251	THR	2.3
1	A	433	PRO	2.3
1	D	456	ASN	2.2
1	C	449	LYS	2.2
1	E	494	GLN	2.2
1	A	372	ARG	2.2
1	C	185	THR	2.2
1	E	439	GLU	2.2
1	C	389	ASN	2.2
1	A	427	PRO	2.2
1	C	321	VAL	2.2
1	D	373	VAL	2.2
1	C	415	CYS	2.2
1	A	418	GLY	2.2
1	C	188	GLY	2.2
1	C	490	LYS	2.2
1	D	321	VAL	2.1
1	B	362	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	364	THR	2.1
1	A	458	TRP	2.1
1	E	458	TRP	2.1
1	A	477	ALA	2.1
1	B	235	SER	2.1
1	E	448	GLN	2.1
1	D	444	VAL	2.1
1	D	453	ASN	2.1
1	B	217	GLY	2.1
1	D	499	GLU	2.1
1	A	250	GLN	2.1
1	D	299	VAL	2.1
1	B	294	ARG	2.1
1	A	368	ALA	2.1
1	D	440	GLU	2.1
1	C	441	MET	2.0
1	C	440	GLU	2.0
1	A	210	SER	2.0
1	D	421	HIS	2.0
1	B	366	ASP	2.0
1	B	438	VAL	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($\text{\AA}^2$)	Q<0.9
2	SO4	C	5	5/5	0.65	0.20	118,119,119,120	0
2	SO4	D	15	5/5	0.66	0.18	111,111,112,112	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	SO4	A	18	5/5	0.77	0.13	104,104,105,105	0
2	SO4	C	4	5/5	0.77	0.13	100,101,102,102	0
2	SO4	E	20	5/5	0.77	0.13	109,109,110,110	0
2	SO4	B	12	5/5	0.80	0.16	98,99,100,100	0
2	SO4	D	14	5/5	0.82	0.12	109,109,109,110	0
2	SO4	D	13	5/5	0.83	0.20	93,93,94,94	0
2	SO4	B	6	5/5	0.84	0.14	99,99,100,100	0
2	SO4	A	21	5/5	0.84	0.10	123,123,123,123	0
2	SO4	C	10	5/5	0.86	0.15	98,99,100,100	0
2	SO4	E	2	5/5	0.87	0.10	111,111,113,113	0
2	SO4	B	11	5/5	0.87	0.16	99,100,100,101	0
2	SO4	A	9	5/5	0.89	0.17	111,112,112,112	0
2	SO4	E	1	5/5	0.89	0.16	93,94,94,95	0

6.5 Other polymers [i](#)

There are no such residues in this entry.