



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 12:28 AM GMT

PDB ID : 2AKW
Title : Crystal Structure of T.Thermophilus Phenylalanyl-tRNA synthetase complexed with p-Cl-Phenylalanine
Authors : Kotik-Kogan, O.M.; Moor, N.A.; Tworowski, D.E.; Safro, M.G.
Deposited on : 2005-08-04
Resolution : 2.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

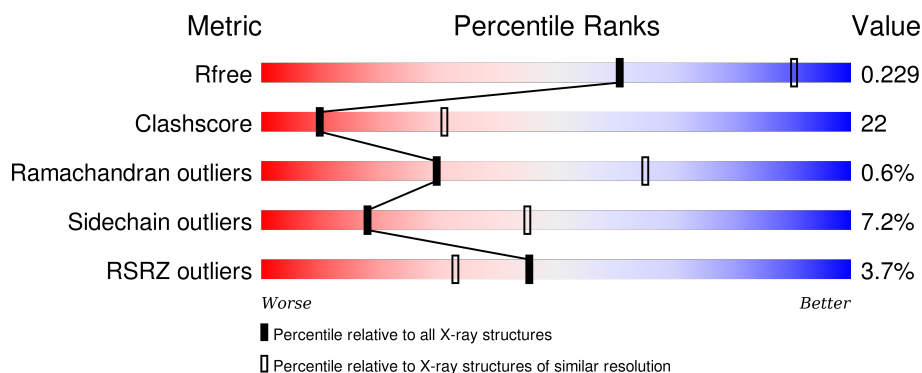
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	266	
2	B	785	

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
4	SO4	B	786	-	X	X	-

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 8466 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 Phenylalanyl-tRNA synthetase alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	266	Total	C	N	O	S	0	0	0
			2123	1388	363	365	7			

- Molecule 2 is a protein called Phenylalanyl-tRNA synthetase beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	785	Total	C	N	O	S	0	0	0
			6127	3925	1091	1101	10			

- Molecule 3 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

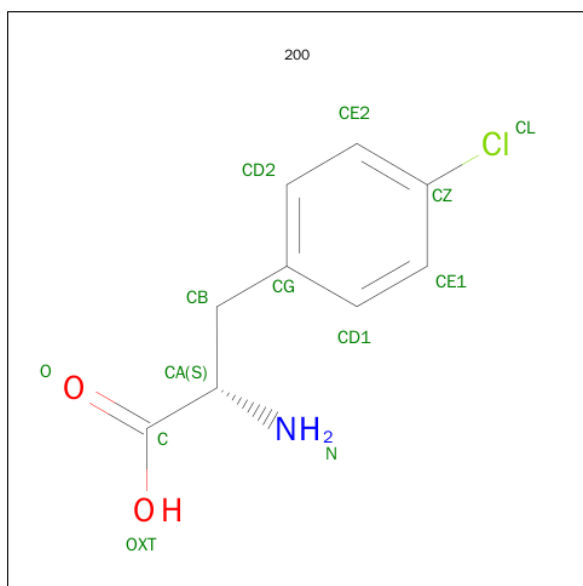
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mn	0	0
			1	1		

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

- Molecule 5 is 4-CHLORO-L-PHENYLALANINE (three-letter code: 200) (formula: $C_9H_9ClNO_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	Cl	N	O	0	0
			13	9	1	1	2		

- Molecule 6 is water.

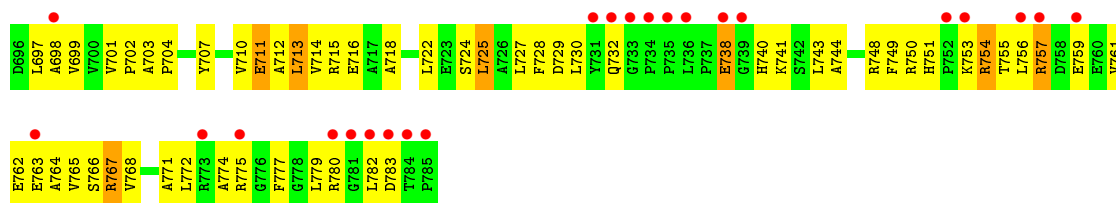
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	41	Total	O	0	0
			41	41		
6	B	156	Total	O	0	0
			156	156		

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

- Chain A:
-
- 2% 66% 32%
- Chain A is a horizontal bar chart showing a distribution of 66% green and 32% yellow, with a 2% red segment at the start. A small red dot is visible at the end of the bar.

- Chain B: 4% 59% 37%

Item	Color	Label
R1	Green	P141
R2	Green	T144
R3	Green	S147
R4	Green	E153
R5	Green	V154
R6	Green	L158
R7	Green	M163
R8	Green	L168
R9	Green	G169
R10	Green	L170
R11	Green	V268
R12	Green	L173
R13	Green	D176
R14	Green	L177
R15	Green	H178
R16	Green	A179
R17	Green	L180
R18	Green	G182
R19	Green	E183
R20	Green	L184
R21	Green	V185
R22	Green	E186
R23	Green	L191
R24	Green	K192
R25	Green	A193
R26	Green	E194
R27	Green	L198
R28	Green	K203
R29	Green	V204
R30	Green	E205
R31	Green	G209
R32	Green	A210
R33	Green	P211
R34	Green	E212
R35	Green	L118
R36	Green	S119
R37	Green	P120
R38	Green	R121
R39	Green	E122
R40	Green	E127
R41	Green	L132
R42	Green	L133
R43	Green	E137
R44	Green	V244
R45	Green	L245
R46	Green	E246
R47	Green	L247
R48	Green	E248
R49	Green	L249
R50	Green	E250
R51	Green	L251
R52	Green	E252
R53	Green	L253
R54	Green	E254
R55	Green	L255
R56	Green	E256
R57	Green	L257
R58	Green	E258
R59	Green	L259
R60	Green	E260
R61	Green	L261
R62	Green	E262
R63	Green	L263
R64	Green	E264
R65	Green	L265
R66	Green	E266
R67	Green	L267
R68	Green	E268
R69	Green	L269
R70	Green	E270
R71	Green	L271
R72	Green	E272
R73	Green	L273
R74	Green	E274
R75	Green	L275
R76	Green	E276
R77	Green	L277
R78	Green	E278
R79	Green	L279
R80	Green	E280
R81	Green	L281
R82	Green	E282
R83	Green	L283
R84	Green	E284
R85	Green	L285
R86	Green	E286
R87	Green	L287
R88	Green	E288
R89	Green	L289
R90	Green	E290
R91	Green	L291
R92	Green	E292
R93	Green	L293
R94	Green	E294
R95	Green	L295
R96	Green	E296
R97	Green	L297
R98	Green	E298
R99	Green	L299
R100	Green	E300



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	172.98Å 172.98Å 138.51Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	9.99 – 2.80 29.96 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.3 (9.99-2.80) 99.3 (29.96-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.98 (at 2.80Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.229 , 0.234 0.224 , 0.229	Depositor DCC
R_{free} test set	2844 reflections (5.04%)	DCC
Wilson B-factor (Å ²)	49.2	Xtriage
Anisotropy	0.462	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 62.2	EDS
Estimated twinning fraction	0.012 for -h,-k,l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	1 of 58657 reflections (0.002%)	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	8466	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.60% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: 200, MN, 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	0.41	0/2191	0.63	0/2971
2	B	0.42	1/6280 (0.0%)	0.70	6/8536 (0.1%)
All	All	0.42	1/8471 (0.0%)	0.69	6/11507 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	99	LEU	N-CA	14.35	1.75	1.46

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	99	LEU	N-CA-CB	-17.22	75.95	110.40
2	B	98	GLY	C-N-CA	-9.59	97.72	121.70
2	B	99	LEU	N-CA-C	9.38	136.32	111.00
2	B	38	VAL	N-CA-C	6.68	129.05	111.00
2	B	133	LEU	CA-CB-CG	5.35	127.61	115.30
2	B	332	ALA	N-CA-C	-5.09	97.26	111.00

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	2123	0	2075	87	0
2	B	6127	0	6180	283	0
3	A	1	0	0	0	0
4	B	5	0	0	2	0
5	A	13	0	9	2	0
6	A	41	0	0	1	0
6	B	156	0	0	0	0
All	All	8466	0	8264	365	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 22.

All (365) 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:B:99:LEU:N	2:B:99:LEU:CA	1.75	1.45
1:A:167:GLU:OE2	1:A:301:LEU:HD21	1.10	1.25
2:B:99:LEU:N	2:B:99:LEU:CB	2.02	1.20
1:A:167:GLU:OE2	1:A:301:LEU:CD2	2.05	1.03
2:B:282:ARG:HH11	2:B:282:ARG:HB3	1.25	1.01
2:B:198:LEU:HD12	2:B:393:LEU:HD13	1.43	0.99
1:A:183:GLN:HB2	1:A:222:LEU:HD22	1.44	0.98
2:B:98:GLY:C	2:B:99:LEU:CA	2.33	0.95
2:B:467:GLN:HE21	2:B:467:GLN:HA	1.30	0.95
1:A:165:LEU:HD12	1:A:301:LEU:HD23	1.49	0.95
2:B:656:HIS:HB3	2:B:659:ILE:HD13	1.51	0.89
2:B:192:LYS:H	2:B:381:GLN:HE22	1.21	0.87
2:B:557:LYS:HG2	2:B:665:LEU:HD21	1.58	0.85
2:B:407:ARG:NH2	4:B:786:SO4:O1	2.08	0.85
2:B:713:LEU:HD11	2:B:775:ARG:HG3	1.57	0.85
2:B:176:ASP:OD2	2:B:465:ARG:NH2	2.10	0.84
2:B:99:LEU:HB2	2:B:99:LEU:N	1.91	0.84
2:B:602:ARG:HG3	2:B:602:ARG:HH11	1.46	0.80
2:B:782:LEU:HD23	2:B:783:ASP:N	1.95	0.80
2:B:282:ARG:NH1	2:B:282:ARG:HB3	1.96	0.79
2:B:596:LEU:HB2	2:B:599:ALA:HB3	1.66	0.78
2:B:80:ASN:H	2:B:80:ASN:HD22	1.33	0.77
2:B:516:MET:HE3	2:B:546:THR:H	1.50	0.76
2:B:600:LYS:HD3	2:B:600:LYS:N	2.00	0.75
1:A:160:ARG:HH21	2:B:579:GLU:HB3	1.52	0.75
2:B:214:THR:HG22	2:B:394:GLU:HG3	1.69	0.75
2:B:461:GLU:O	2:B:465:ARG:HG2	1.87	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:767:ARG:N	2:B:767:ARG:HE	1.85	0.74
2:B:710:VAL:HG11	2:B:743:LEU:HD12	1.68	0.74
2:B:649:VAL:HG23	2:B:673:LEU:HD22	1.70	0.74
1:A:179:THR:OG1	1:A:220:GLU:HG2	1.88	0.74
2:B:255:GLU:OE2	2:B:375:ARG:HD2	1.89	0.73
2:B:98:GLY:O	2:B:99:LEU:CA	2.37	0.73
2:B:56:ILE:HB	2:B:59:THR:OG1	1.89	0.72
2:B:427:ILE:HD12	2:B:466:ILE:CG2	2.19	0.72
2:B:693:ALA:HB3	2:B:749:PHE:HB2	1.71	0.71
2:B:374:ARG:HH11	2:B:374:ARG:HG2	1.55	0.71
2:B:407:ARG:HD3	2:B:456:GLU:OE2	1.90	0.71
1:A:317:LEU:O	1:A:317:LEU:HD12	1.90	0.71
2:B:764:ALA:HA	2:B:767:ARG:HG2	1.71	0.71
2:B:761:VAL:O	2:B:765:VAL:HG13	1.90	0.71
1:A:198:VAL:HG13	1:A:220:GLU:HB2	1.73	0.71
2:B:604:SER:HA	2:B:608:LEU:HD22	1.72	0.70
1:A:280:LEU:HD21	1:A:322:LEU:HD23	1.71	0.70
2:B:192:LYS:N	2:B:381:GLN:HE22	1.89	0.70
2:B:99:LEU:CB	2:B:99:LEU:H	2.05	0.69
2:B:294:HIS:CE1	2:B:296:GLU:HB2	2.28	0.69
2:B:490:ALA:HB3	2:B:491:PRO:HD3	1.75	0.69
2:B:279:GLU:HG2	2:B:295:PRO:HD3	1.73	0.68
1:A:169:VAL:HG22	1:A:170:GLU:H	1.59	0.68
1:A:165:LEU:HD11	1:A:303:LEU:HD11	1.76	0.68
2:B:427:ILE:HD12	2:B:466:ILE:HG21	1.77	0.67
2:B:697:LEU:O	2:B:697:LEU:HD12	1.94	0.67
2:B:763:GLU:OE2	2:B:767:ARG:HD2	1.94	0.67
2:B:519:GLU:HB3	2:B:523:ARG:NH1	2.11	0.66
2:B:63:ARG:HD2	2:B:73:GLU:OE2	1.96	0.66
2:B:631:PHE:HB2	2:B:634:LEU:HD12	1.77	0.66
2:B:413:ARG:NH2	4:B:786:SO4:O4	2.29	0.65
1:A:271:TRP:CZ3	1:A:274:GLY:HA3	2.31	0.65
2:B:701:VAL:HG13	2:B:702:PRO:HD2	1.79	0.65
1:A:329:ILE:HD11	1:A:346:PHE:HZ	1.61	0.65
2:B:176:ASP:CG	2:B:465:ARG:HH22	2.00	0.65
2:B:258:GLN:HE22	2:B:369:GLN:NE2	1.94	0.65
2:B:701:VAL:HG22	2:B:777:PHE:CD1	2.32	0.64
1:A:210:ALA:HA	1:A:331:ASP:OD1	1.98	0.64
2:B:28:LEU:HD13	2:B:176:ASP:HB3	1.80	0.64
2:B:277:ALA:O	2:B:295:PRO:HA	1.98	0.64
2:B:702:PRO:HA	2:B:740:HIS:HA	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:703:ALA:N	2:B:704:PRO:HD2	2.13	0.63
1:A:160:ARG:NH2	2:B:579:GLU:HB3	2.12	0.63
1:A:169:VAL:HG22	1:A:170:GLU:N	2.13	0.63
2:B:732:GLN:HB3	2:B:741:LYS:HB3	1.81	0.62
2:B:751:HIS:HB3	2:B:754:ARG:O	1.98	0.62
1:A:329:ILE:HD11	1:A:346:PHE:CZ	2.34	0.62
1:A:109:GLU:O	1:A:113:ILE:HG12	2.00	0.62
1:A:165:LEU:CD1	1:A:301:LEU:HD23	2.28	0.62
2:B:99:LEU:HB3	2:B:99:LEU:N	2.13	0.62
2:B:698:ALA:HB3	2:B:780:ARG:HB3	1.81	0.62
2:B:49:ARG:HD2	2:B:137:GLU:HG3	1.82	0.62
2:B:583:THR:HG22	2:B:675:LEU:HD12	1.81	0.62
1:A:300:ARG:HB2	1:A:300:ARG:NH1	2.14	0.61
2:B:353:ARG:C	2:B:353:ARG:HD3	2.21	0.61
1:A:113:ILE:HD12	1:A:243:ALA:HB1	1.83	0.61
2:B:457:GLU:HA	2:B:460:VAL:HG13	1.81	0.61
2:B:582:GLU:OE2	2:B:584:HIS:HE1	1.83	0.61
2:B:224:ALA:N	2:B:244:ASN:ND2	2.48	0.61
2:B:80:ASN:HD21	2:B:132:LEU:H	1.47	0.60
2:B:62:LYS:NZ	2:B:62:LYS:HB2	2.15	0.60
1:A:308:ARG:HE	1:A:308:ARG:HA	1.66	0.60
2:B:530:ARG:HD2	2:B:579:GLU:H	1.66	0.60
1:A:223:VAL:HG12	1:A:228:ILE:HD13	1.83	0.60
2:B:782:LEU:HD23	2:B:783:ASP:HB2	1.84	0.60
2:B:98:GLY:O	2:B:99:LEU:HA	2.00	0.60
2:B:557:LYS:HA	2:B:560:LEU:HD12	1.83	0.60
2:B:643:LEU:HD12	2:B:646:GLY:O	2.02	0.60
2:B:80:ASN:H	2:B:80:ASN:ND2	2.00	0.60
2:B:282:ARG:HH11	2:B:282:ARG:CB	2.10	0.60
2:B:767:ARG:CA	2:B:767:ARG:HE	2.14	0.60
2:B:44:GLY:HA3	2:B:94:THR:OG1	2.02	0.59
2:B:589:LEU:HD21	2:B:608:LEU:HD23	1.84	0.59
2:B:530:ARG:HB2	2:B:530:ARG:NH1	2.17	0.59
2:B:265:LEU:HD23	2:B:268:VAL:HG21	1.84	0.59
2:B:467:GLN:NE2	2:B:467:GLN:HA	2.11	0.58
2:B:209:GLY:C	2:B:211:PRO:HD3	2.23	0.58
2:B:732:GLN:HB2	2:B:740:HIS:O	2.04	0.58
2:B:605:GLY:HA2	2:B:669:HIS:CD2	2.39	0.57
2:B:256:ARG:NH2	2:B:375:ARG:HG3	2.18	0.57
2:B:520:ASP:HA	2:B:523:ARG:HB2	1.86	0.57
2:B:589:LEU:HD12	2:B:590:PHE:H	1.70	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:101:GLN:NE2	2:B:101:GLN:N	2.52	0.57
1:A:155:THR:HB	2:B:534:LEU:HD21	1.87	0.57
2:B:223:VAL:HA	2:B:244:ASN:HD22	1.69	0.57
2:B:690:HIS:HB3	2:B:691:PRO:HD2	1.85	0.57
2:B:688:SER:HB3	2:B:750:ARG:HD3	1.87	0.57
1:A:271:TRP:HZ3	1:A:276:LYS:HE2	1.69	0.57
2:B:587:GLY:HA3	2:B:671:PHE:CE1	2.39	0.57
1:A:162:GLU:O	1:A:185:ARG:NH2	2.38	0.57
1:A:298:ARG:NH1	1:A:304:PRO:O	2.37	0.57
1:A:165:LEU:HB2	1:A:167:GLU:OE1	2.04	0.57
1:A:223:VAL:HG12	1:A:228:ILE:CD1	2.35	0.57
2:B:762:GLU:O	2:B:765:VAL:HG22	2.05	0.56
2:B:224:ALA:H	2:B:244:ASN:ND2	2.03	0.56
2:B:212:HIS:HE1	2:B:394:GLU:OE2	1.89	0.56
2:B:530:ARG:HH11	2:B:530:ARG:HB2	1.70	0.56
2:B:692:ALA:HB2	2:B:750:ARG:NH1	2.21	0.56
2:B:593:GLY:HA3	2:B:604:SER:HB3	1.88	0.56
2:B:596:LEU:HB2	2:B:599:ALA:CB	2.34	0.56
2:B:141:PRO:O	2:B:144:THR:HG23	2.06	0.56
1:A:349:VAL:HG12	1:A:350:LEU:HD23	1.87	0.56
2:B:120:PRO:HG3	2:B:133:LEU:HD13	1.87	0.56
2:B:701:VAL:CG1	2:B:702:PRO:HD2	2.36	0.55
2:B:163:ASN:O	2:B:452:ASP:HB3	2.07	0.55
1:A:292:GLN:HA	1:A:308:ARG:HH22	1.71	0.55
2:B:563:ASP:C	2:B:564:ARG:HD2	2.26	0.55
1:A:261:VAL:HG11	5:A:999:200:CL	2.44	0.55
1:A:85:ARG:HD2	1:A:85:ARG:N	2.21	0.55
2:B:49:ARG:CD	2:B:137:GLU:HG3	2.37	0.55
2:B:264:ASP:OD1	2:B:266:ARG:HG3	2.07	0.55
2:B:56:ILE:HD11	2:B:63:ARG:HB2	1.89	0.55
1:A:182:MET:HG2	1:A:198:VAL:HG21	1.88	0.54
2:B:536:PRO:HB3	2:B:542:ALA:HA	1.87	0.54
2:B:602:ARG:NH1	2:B:602:ARG:HG3	2.17	0.54
2:B:578:ARG:O	2:B:579:GLU:HB2	2.08	0.54
1:A:324:MET:HG2	1:A:329:ILE:HB	1.89	0.54
1:A:178:HIS:HB2	1:A:218:GLN:HE22	1.73	0.54
2:B:516:MET:SD	2:B:529:PRO:HG3	2.47	0.54
2:B:509:GLU:HB2	2:B:571:PHE:CE1	2.42	0.54
1:A:87:ASP:O	1:A:90:LEU:HB2	2.07	0.54
2:B:203:LYS:HE3	2:B:205:GLU:OE2	2.06	0.54
2:B:755:THR:HG22	2:B:756:LEU:N	2.23	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:554:ARG:HG2	2:B:554:ARG:HH11	1.72	0.53
2:B:768:VAL:O	2:B:772:LEU:HB2	2.08	0.53
2:B:730:LEU:HD13	2:B:743:LEU:HD23	1.91	0.53
2:B:642:VAL:C	2:B:643:LEU:HD22	2.29	0.53
2:B:519:GLU:HB3	2:B:523:ARG:HH12	1.72	0.53
2:B:710:VAL:O	2:B:714:VAL:HG23	2.08	0.53
2:B:368:GLY:O	2:B:371:PRO:HD2	2.09	0.52
1:A:237:ILE:HG22	1:A:251:VAL:HG11	1.90	0.52
2:B:604:SER:HA	2:B:608:LEU:HB2	1.92	0.52
1:A:252:ARG:NH2	1:A:279:GLU:OE2	2.43	0.52
1:A:174:LEU:HD12	1:A:174:LEU:C	2.30	0.52
2:B:282:ARG:HH12	2:B:290:GLU:HG3	1.74	0.52
2:B:258:GLN:HE22	2:B:369:GLN:HE21	1.58	0.52
2:B:49:ARG:CG	2:B:137:GLU:HG3	2.40	0.52
2:B:552:LEU:O	2:B:555:VAL:HG22	2.10	0.52
2:B:718:ALA:CB	2:B:722:LEU:HD22	2.40	0.52
2:B:409:GLU:OE1	2:B:413:ARG:HD3	2.10	0.51
2:B:408:PRO:HG2	2:B:421:GLU:HG3	1.90	0.51
2:B:178:HIS:CD2	2:B:430:ARG:HH12	2.28	0.51
2:B:730:LEU:HD13	2:B:743:LEU:CD2	2.39	0.51
2:B:178:HIS:O	2:B:430:ARG:NH1	2.43	0.51
2:B:474:LEU:HD12	2:B:474:LEU:N	2.25	0.51
2:B:656:HIS:HE1	2:B:658:GLU:HG3	1.75	0.51
1:A:102:PRO:HG3	1:A:346:PHE:CD1	2.46	0.51
1:A:113:ILE:HD12	1:A:243:ALA:CB	2.40	0.51
1:A:174:LEU:HD12	1:A:174:LEU:O	2.10	0.51
1:A:188:VAL:HG12	1:A:294:VAL:HG13	1.91	0.51
2:B:600:LYS:HG2	2:B:601:GLU:OE2	2.10	0.51
2:B:49:ARG:HD2	2:B:137:GLU:CG	2.41	0.51
1:A:256:VAL:HG12	1:A:265:ALA:C	2.31	0.51
2:B:49:ARG:HG3	2:B:137:GLU:HG3	1.93	0.51
2:B:702:PRO:C	2:B:704:PRO:HD2	2.30	0.51
2:B:718:ALA:HB3	2:B:722:LEU:HD22	1.93	0.51
2:B:407:ARG:HG3	2:B:441:THR:HB	1.92	0.50
2:B:588:LEU:HD23	2:B:588:LEU:C	2.32	0.50
2:B:657:PRO:O	2:B:661:GLN:OE1	2.29	0.50
2:B:757:ARG:HG2	2:B:757:ARG:HH11	1.77	0.50
2:B:697:LEU:HD12	2:B:697:LEU:C	2.31	0.50
1:A:201:ARG:HD2	1:A:336:PHE:HZ	1.77	0.49
1:A:191:THR:HG23	2:B:484:ASP:OD2	2.12	0.49
2:B:693:ALA:O	2:B:748:ARG:HA	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:583:THR:CG2	2:B:675:LEU:HD12	2.43	0.49
2:B:690:HIS:CE1	2:B:753:LYS:O	2.65	0.49
1:A:271:TRP:CZ3	1:A:325:LEU:HD11	2.47	0.49
2:B:762:GLU:OE2	2:B:783:ASP:OD2	2.31	0.49
1:A:269:VAL:CG1	1:A:280:LEU:HD12	2.42	0.49
2:B:326:GLU:CD	2:B:326:GLU:H	2.16	0.49
2:B:699:VAL:CG1	2:B:772:LEU:HD11	2.43	0.49
2:B:374:ARG:NH1	2:B:374:ARG:HG2	2.26	0.49
2:B:701:VAL:HG22	2:B:777:PHE:HD1	1.78	0.49
2:B:638:VAL:HB	2:B:654:ALA:HB3	1.95	0.49
1:A:269:VAL:HG13	1:A:280:LEU:HD12	1.96	0.48
1:A:113:ILE:CD1	1:A:243:ALA:HB1	2.43	0.48
1:A:108:ARG:O	1:A:112:GLU:HG2	2.13	0.48
2:B:610:LYS:NZ	2:B:626:VAL:HB	2.28	0.48
1:A:85:ARG:HH11	1:A:85:ARG:HG3	1.79	0.48
1:A:85:ARG:NH1	1:A:85:ARG:HG3	2.28	0.48
2:B:767:ARG:NE	2:B:767:ARG:CA	2.76	0.48
1:A:190:HIS:HB3	2:B:484:ASP:OD1	2.14	0.48
2:B:578:ARG:O	2:B:579:GLU:CB	2.62	0.48
2:B:755:THR:HG22	2:B:756:LEU:H	1.79	0.48
1:A:179:THR:OG1	1:A:220:GLU:CG	2.61	0.47
2:B:357:SER:O	2:B:361:GLU:HG3	2.14	0.47
2:B:362:ARG:HG2	2:B:362:ARG:HH11	1.79	0.47
2:B:729:ASP:HB3	2:B:744:ALA:CB	2.44	0.47
1:A:350:LEU:HD22	1:A:350:LEU:N	2.30	0.47
2:B:341:VAL:HG12	2:B:345:LYS:HE3	1.96	0.47
2:B:300:ILE:O	2:B:311:LEU:HB2	2.14	0.47
2:B:775:ARG:NH1	2:B:777:PHE:HE2	2.11	0.47
2:B:224:ALA:HB1	2:B:225:PRO:CD	2.45	0.47
2:B:489:GLU:HG3	2:B:493:ARG:HD2	1.97	0.47
2:B:604:SER:HA	2:B:608:LEU:CD2	2.44	0.47
2:B:516:MET:HE3	2:B:546:THR:N	2.24	0.47
1:A:101:HIS:CG	1:A:102:PRO:HD2	2.50	0.47
2:B:224:ALA:N	2:B:244:ASN:HD22	2.13	0.47
2:B:286:LEU:HD21	2:B:323:GLU:HG3	1.96	0.47
2:B:478:ALA:O	2:B:479:PHE:HB3	2.14	0.47
2:B:549:PHE:CD1	2:B:549:PHE:C	2.88	0.47
2:B:775:ARG:CZ	2:B:775:ARG:HB3	2.43	0.47
2:B:564:ARG:N	2:B:564:ARG:HD2	2.30	0.47
2:B:724:SER:H	2:B:748:ARG:HB2	1.80	0.47
2:B:496:GLN:O	2:B:500:GLU:HG3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:711:GLU:CD	2:B:715:ARG:HH12	2.18	0.46
2:B:695:ARG:HD2	2:B:765:VAL:HG11	1.97	0.46
2:B:519:GLU:HG3	2:B:522:ARG:NH2	2.30	0.46
2:B:763:GLU:O	2:B:766:SER:HB2	2.15	0.46
2:B:557:LYS:CG	2:B:665:LEU:HD21	2.38	0.46
1:A:271:TRP:CE3	1:A:274:GLY:HA3	2.50	0.46
2:B:235:PHE:CZ	2:B:241:PRO:HD2	2.50	0.46
2:B:515:PHE:CE1	2:B:533:LEU:HD21	2.50	0.46
1:A:180:SER:N	1:A:181:PRO:HD2	2.30	0.46
2:B:50:VAL:HG12	2:B:83:LYS:HA	1.98	0.46
2:B:771:ALA:HA	2:B:774:ALA:HB3	1.98	0.46
2:B:562:LEU:HD22	2:B:563:ASP:OD1	2.15	0.46
2:B:24:ARG:NE	2:B:182:TYR:OH	2.46	0.46
1:A:133:ASN:HA	1:A:181:PRO:HB3	1.96	0.46
1:A:106:MET:SD	1:A:322:LEU:HD12	2.56	0.46
2:B:296:GLU:HB3	2:B:349:ARG:HH12	1.81	0.46
2:B:344:ARG:O	2:B:348:ARG:HD3	2.16	0.46
2:B:772:LEU:O	2:B:777:PHE:HB2	2.17	0.45
1:A:339:ARG:O	1:A:342:PHE:HB3	2.17	0.45
2:B:368:GLY:C	2:B:371:PRO:HD2	2.36	0.45
2:B:33:ASP:O	2:B:34:ARG:HB2	2.16	0.45
2:B:782:LEU:CD2	2:B:783:ASP:HB2	2.47	0.45
1:A:349:VAL:CG1	1:A:350:LEU:HD23	2.46	0.45
2:B:153:GLU:HG3	2:B:154:VAL:N	2.32	0.45
2:B:121:ARG:HG3	2:B:121:ARG:HH11	1.82	0.45
1:A:208:THR:HG22	1:A:333:ARG:HD3	1.98	0.45
2:B:432:GLY:O	2:B:447:PRO:HG3	2.16	0.45
2:B:210:ALA:HB2	2:B:274:VAL:HG11	1.98	0.45
2:B:698:ALA:O	2:B:779:LEU:HD12	2.16	0.45
2:B:554:ARG:HG2	2:B:554:ARG:NH1	2.30	0.45
2:B:707:TYR:CE1	2:B:727:LEU:HD22	2.51	0.45
1:A:330:PRO:HG2	1:A:334:TYR:HE2	1.82	0.45
2:B:428:LEU:O	2:B:433:CYS:HB2	2.16	0.45
2:B:702:PRO:HB2	2:B:704:PRO:HD2	1.99	0.44
2:B:699:VAL:HG11	2:B:772:LEU:HD11	1.99	0.44
2:B:168:LEU:HA	2:B:168:LEU:HD23	1.85	0.44
2:B:75:VAL:HG23	2:B:111:VAL:HG22	1.99	0.44
2:B:651:PHE:CD1	2:B:651:PHE:C	2.91	0.44
2:B:516:MET:HG2	2:B:517:ASP:N	2.33	0.44
2:B:279:GLU:HG2	2:B:295:PRO:CD	2.46	0.44
1:A:101:HIS:ND1	1:A:102:PRO:HD2	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:62:LYS:HZ3	2:B:62:LYS:HB2	1.81	0.44
2:B:24:ARG:HD2	2:B:182:TYR:HE1	1.83	0.44
1:A:224:VAL:HG12	1:A:225:GLY:N	2.33	0.44
1:A:271:TRP:CZ3	1:A:276:LYS:HE2	2.50	0.44
2:B:369:GLN:CD	2:B:369:GLN:H	2.21	0.44
2:B:652:LEU:HD12	2:B:670:LEU:O	2.18	0.44
2:B:455:LEU:O	2:B:458:ASP:HB2	2.17	0.44
2:B:278:ARG:HB2	2:B:281:GLU:HG3	2.00	0.44
2:B:623:ALA:HB3	2:B:645:GLU:HA	1.99	0.43
2:B:43:ARG:HH11	2:B:43:ARG:HG3	1.82	0.43
2:B:656:HIS:HB3	2:B:659:ILE:CD1	2.35	0.43
2:B:425:ILE:HD11	2:B:442:TYR:CZ	2.53	0.43
1:A:271:TRP:HB2	1:A:278:LEU:HD11	1.99	0.43
1:A:300:ARG:HB2	1:A:300:ARG:HH11	1.82	0.43
2:B:455:LEU:O	2:B:459:LEU:HD22	2.18	0.43
2:B:194:GLU:OE1	2:B:387:ARG:NH2	2.49	0.43
2:B:635:HIS:O	2:B:639:SER:HB2	2.18	0.43
2:B:779:LEU:CD2	2:B:782:LEU:HD12	2.48	0.43
2:B:498:LEU:O	2:B:502:LEU:HG	2.18	0.43
2:B:249:THR:HB	2:B:260:MET:HG3	2.00	0.43
2:B:409:GLU:OE2	2:B:413:ARG:NH1	2.43	0.43
1:A:121:ALA:HA	1:A:197:VAL:O	2.19	0.43
2:B:703:ALA:N	2:B:704:PRO:CD	2.80	0.43
2:B:757:ARG:HD2	2:B:759:GLU:OE1	2.18	0.43
2:B:286:LEU:HD21	2:B:323:GLU:CG	2.49	0.43
2:B:403:ALA:CB	2:B:443:ARG:HD3	2.48	0.43
2:B:695:ARG:NH1	2:B:761:VAL:HG12	2.34	0.43
2:B:762:GLU:CD	2:B:783:ASP:OD2	2.57	0.43
1:A:322:LEU:O	1:A:322:LEU:HD13	2.19	0.43
2:B:405:PRO:HA	2:B:442:TYR:O	2.19	0.43
2:B:707:TYR:OH	2:B:711:GLU:HG3	2.19	0.42
1:A:141:GLU:C	1:A:143:HIS:N	2.73	0.42
1:A:317:LEU:C	1:A:317:LEU:HD12	2.40	0.42
2:B:694:PHE:CD1	2:B:694:PHE:N	2.87	0.42
2:B:43:ARG:HG3	2:B:43:ARG:NH1	2.34	0.42
2:B:222:ARG:O	2:B:222:ARG:HG3	2.19	0.42
2:B:509:GLU:HB2	2:B:571:PHE:CZ	2.54	0.42
1:A:179:THR:C	1:A:181:PRO:HD2	2.40	0.42
2:B:277:ALA:HB2	2:B:299:VAL:HG21	2.02	0.42
1:A:143:HIS:ND1	1:A:144:PRO:HD2	2.34	0.42
2:B:119:SER:OG	2:B:122:GLU:HG3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:221:GLY:HA3	1:A:315:PHE:CZ	2.54	0.42
2:B:184:LEU:HD11	2:B:186:GLU:HG3	2.02	0.42
1:A:329:ILE:CD1	1:A:346:PHE:HZ	2.29	0.42
1:A:258:PHE:CZ	5:A:999:200:HD2	2.55	0.42
1:A:321:ARG:HD3	6:A:1021:HOH:O	2.18	0.42
2:B:192:LYS:H	2:B:381:GLN:NE2	2.03	0.41
2:B:252:VAL:HG11	2:B:260:MET:HE1	2.01	0.41
2:B:101:GLN:CD	2:B:101:GLN:H	2.22	0.41
2:B:560:LEU:HD21	2:B:590:PHE:CZ	2.55	0.41
2:B:665:LEU:HA	2:B:666:PRO:HD3	1.91	0.41
2:B:552:LEU:HA	2:B:555:VAL:HG22	2.02	0.41
2:B:712:ALA:O	2:B:716:GLU:HB2	2.21	0.41
2:B:434:ARG:HB3	2:B:445:THR:HG23	2.01	0.41
2:B:732:GLN:HB3	2:B:741:LYS:CB	2.47	0.41
2:B:728:PHE:CZ	2:B:744:ALA:HB1	2.55	0.41
2:B:90:ALA:HB2	2:B:118:LEU:HD11	2.03	0.41
2:B:99:LEU:HG	2:B:101:GLN:HG2	2.01	0.41
2:B:690:HIS:ND1	2:B:690:HIS:N	2.68	0.41
2:B:652:LEU:HD13	2:B:671:PHE:HB3	2.02	0.41
2:B:311:LEU:HD23	2:B:311:LEU:HA	1.90	0.41
2:B:725:LEU:HD23	2:B:725:LEU:C	2.40	0.41
2:B:551:GLY:O	2:B:555:VAL:HG13	2.21	0.41
2:B:409:GLU:CD	2:B:413:ARG:HD3	2.41	0.41
2:B:255:GLU:OE1	2:B:375:ARG:NH1	2.54	0.41
1:A:195:ARG:HG2	1:A:223:VAL:HG13	2.03	0.41
1:A:165:LEU:HD12	1:A:301:LEU:CD2	2.35	0.41
2:B:214:THR:HA	2:B:393:LEU:O	2.21	0.41
2:B:224:ALA:HB1	2:B:225:PRO:HD2	2.03	0.41
2:B:524:PHE:O	2:B:633:PHE:HB3	2.20	0.41
2:B:600:LYS:HD3	2:B:600:LYS:H	1.80	0.40
1:A:315:PHE:C	1:A:315:PHE:CD1	2.94	0.40
1:A:95:LEU:HD22	1:A:95:LEU:H	1.86	0.40
2:B:531:LEU:O	2:B:532:LEU:HD23	2.21	0.40
2:B:699:VAL:HG12	2:B:701:VAL:HG23	2.03	0.40
1:A:141:GLU:C	1:A:143:HIS:H	2.25	0.40
2:B:548:LEU:H	2:B:672:GLU:CD	2.24	0.40
2:B:590:PHE:CD1	2:B:591:GLY:N	2.89	0.40
2:B:751:HIS:HB2	2:B:756:LEU:CD2	2.51	0.40
2:B:179:ALA:HA	2:B:430:ARG:HB3	2.03	0.40
2:B:533:LEU:HD12	2:B:533:LEU:N	2.36	0.40
2:B:468:GLY:HA3	2:B:470:GLU:OE2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:101:GLN:HE21	2:B:101:GLN:N	2.18	0.40
2:B:557:LYS:HG2	2:B:665:LEU:CD2	2.39	0.40
2:B:601:GLU:H	2:B:601:GLU:CD	2.24	0.40
2:B:575:ARG:HD2	2:B:583:THR:OG1	2.21	0.40
1:A:308:ARG:HE	1:A:308:ARG:CA	2.33	0.40
2:B:682:LEU:HD12	2:B:683:ALA:H	1.87	0.40
2:B:313:LEU:HD22	2:B:346:THR:HG21	2.03	0.40
2:B:559:ASN:O	2:B:563:ASP:O	2.39	0.40
2:B:121:ARG:HG3	2:B:121:ARG:NH1	2.37	0.40
2:B:180:LEU:HA	2:B:180:LEU:HD12	1.95	0.40

There are no symmetry-related clashes.

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	264/266 (99%)	249 (94%)	14 (5%)	1 (0%)	39	74
2	B	783/785 (100%)	725 (93%)	53 (7%)	5 (1%)	30	65
All	All	1047/1051 (100%)	974 (93%)	67 (6%)	6 (1%)	30	65

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	349	VAL
2	B	244	ASN
2	B	578	ARG
2	B	738	GLU
2	B	725	LEU
2	B	568	ALA

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	214/214 (100%)	205 (96%)	9 (4%)	36	71
2	B	630/630 (100%)	578 (92%)	52 (8%)	14	38
All	All	844/844 (100%)	783 (93%)	61 (7%)	18	45

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	85	ARG
1	A	178	HIS
1	A	198	VAL
1	A	201	ARG
1	A	260	PHE
1	A	299	GLU
1	A	301	LEU
1	A	308	ARG
1	A	326	ARG
2	B	32	THR
2	B	34	ARG
2	B	37	ARG
2	B	60	ARG
2	B	74	VAL
2	B	80	ASN
2	B	83	LYS
2	B	89	LEU
2	B	101	GLN
2	B	111	VAL
2	B	127	GLU
2	B	147	SER
2	B	158	LEU
2	B	170	LEU
2	B	171	LEU
2	B	173	LEU
2	B	180	LEU
2	B	191	LEU

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Mol	Chain	Res	Type
2	B	276	ARG
2	B	282	ARG
2	B	283	LEU
2	B	286	LEU
2	B	298	LEU
2	B	322	SER
2	B	323	GLU
2	B	325	ARG
2	B	333	LEU
2	B	362	ARG
2	B	375	ARG
2	B	438	GLU
2	B	441	THR
2	B	443	ARG
2	B	445	THR
2	B	460	VAL
2	B	465	ARG
2	B	467	GLN
2	B	470	GLU
2	B	505	LEU
2	B	549	PHE
2	B	571	PHE
2	B	575	ARG
2	B	576	VAL
2	B	578	ARG
2	B	600	LYS
2	B	609	LEU
2	B	619	ARG
2	B	711	GLU
2	B	713	LEU
2	B	738	GLU
2	B	754	ARG
2	B	757	ARG
2	B	767	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	120	GLN
1	A	183	GLN
1	A	207	GLN
1	A	218	GLN

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Mol	Chain	Res	Type
2	B	54	HIS
2	B	80	ASN
2	B	101	GLN
2	B	178	HIS
2	B	212	HIS
2	B	231	GLN
2	B	244	ASN
2	B	258	GLN
2	B	350	HIS
2	B	381	GLN
2	B	467	GLN
2	B	584	HIS
2	B	661	GLN
2	B	732	GLN
2	B	746	HIS

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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 for Mogul analysis.

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
5	200	A	999	-	10,13,13	2.14	6 (60%)	11,17,17	0.61	0
4	SO4	B	786	-	4,4,4	4.28	4 (100%)	6,6,6	2.40	2 (33%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	200	A	999	-	-	0/4/8/8	0/1/1/1
4	SO4	B	786	-	-	0/0/0/0	0/0/0/0

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	786	SO4	O3-S	-4.99	1.29	1.47
4	B	786	SO4	O2-S	-3.65	1.34	1.47
5	A	999	200	CE1-CD1	2.31	1.42	1.38
5	A	999	200	CE1-CZ	2.32	1.42	1.38
5	A	999	200	CE2-CD2	2.50	1.43	1.38
5	A	999	200	CD2-CG	2.57	1.44	1.38
5	A	999	200	CE2-CZ	2.85	1.43	1.38
5	A	999	200	CD1-CG	3.57	1.46	1.38
4	B	786	SO4	O1-S	3.88	1.60	1.47
4	B	786	SO4	O4-S	4.49	1.63	1.47

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	786	SO4	O2-S-O1	-5.22	92.94	109.50
4	B	786	SO4	O3-S-O2	2.13	129.97	110.19

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	999	200	2	0
4	B	786	SO4	2	0

5.7 Other polymers

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

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	266/266 (100%)	-0.23	4 (1%) 76 68	25, 41, 73, 86	0
2	B	785/785 (100%)	-0.12	35 (4%) 37 26	22, 46, 87, 87	0
All	All	1051/1051 (100%)	-0.15	39 (3%) 45 33	22, 44, 86, 87	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	782	LEU	6.8
2	B	783	ASP	6.1
2	B	781	GLY	6.0
2	B	739	GLY	4.9
2	B	98	GLY	4.7
2	B	736	LEU	4.5
2	B	732	GLN	4.1
2	B	784	THR	4.1
2	B	785	PRO	4.1
2	B	731	TYR	4.0
2	B	759	GLU	3.3
2	B	756	LEU	3.3
1	A	350	LEU	3.2
2	B	738	GLU	3.0
1	A	167	GLU	3.0
2	B	733	GLY	3.0
2	B	698	ALA	2.8
2	B	101	GLN	2.8
2	B	780	ARG	2.7
2	B	99	LEU	2.7
2	B	663	LEU	2.7
2	B	681	PRO	2.6
2	B	279	GLU	2.5
2	B	689	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
2	B	753	LYS	2.4
2	B	734	PRO	2.4
1	A	207	GLN	2.4
2	B	661	GLN	2.3
2	B	752	PRO	2.3
2	B	763	GLU	2.3
1	A	143	HIS	2.3
2	B	773	ARG	2.2
2	B	100	GLY	2.2
2	B	775	ARG	2.2
2	B	735	PRO	2.1
2	B	757	ARG	2.1
2	B	34	ARG	2.1
2	B	692	ALA	2.1
2	B	679	ASP	2.1

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
5	200	A	999	13/13	0.88	0.18	-0.04	8,12,18,54	0
3	MN	A	901	1/1	0.82	0.11	-1.70	42,42,42,42	0
4	SO4	B	786	5/5	0.94	0.34	-	7,7,7,18	0

6.5 Other polymers [i](#)

There are no such residues in this entry.