



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:59 PM UTC

PDB ID : 3JV6 / pdb_00003jv6
Title : Crystal structure of the dimerization domains p52 and RelB
Authors : Vu, D.; Huang, D.B.; Ghosh, G.
Deposited on : 2009-09-15
Resolution : 2.78 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

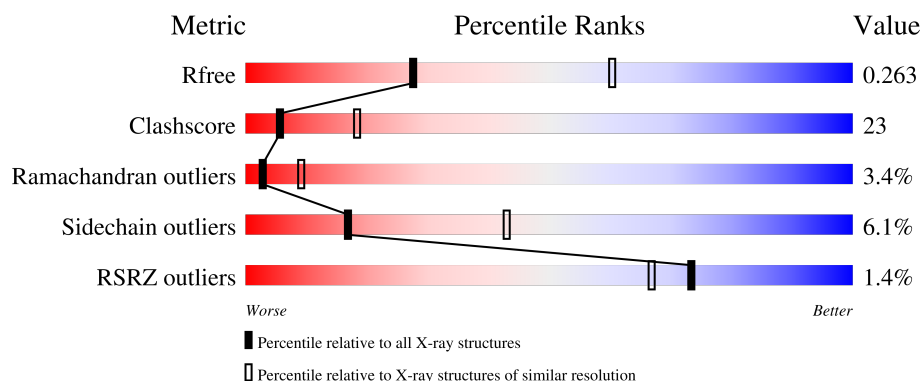
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.78 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.



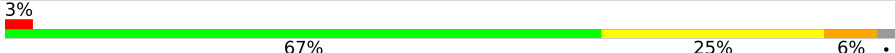
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	5248 (2.80-2.76)
Clashscore	190562	5693 (2.80-2.76)
Ramachandran outliers	187476	5590 (2.80-2.76)
Sidechain outliers	187428	5592 (2.80-2.76)
RSRZ outliers	180081	5251 (2.80-2.76)

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	101	% 59% 36% 5%
1	C	101	51% 42% 7%
1	E	101	% 50% 44% 6%
2	B	107	2% 55% 32% 13%
2	D	107	2% 59% 36% • •

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Mol	Chain	Length	Quality of chain
2	F	107	 A horizontal bar chart showing the quality of chain F. The bar is divided into four segments: a small red segment at the beginning labeled '3%', followed by a large green segment labeled '67%', then a yellow segment labeled '25%', and a small orange segment at the end labeled '6%'. A small grey dot is visible at the far right end of the bar.

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5191 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 Transcription factor RelB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	101	Total	C	N	O	S	0	0	0
			800	507	132	157	4			
1	C	101	Total	C	N	O	S	0	0	0
			800	507	132	157	4			
1	E	101	Total	C	N	O	S	0	0	0
			800	507	132	157	4			

- Molecule 2 is a protein called Nuclear factor NF-kappa-B p100 subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	107	Total	C	N	O	S	0	0	0
			875	555	150	167	3			
2	D	106	Total	C	N	O	S	0	0	0
			867	551	149	164	3			
2	F	105	Total	C	N	O	S	0	0	0
			858	546	148	161	3			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	328	VAL	LEU	conflict	UNP Q9WTK5
D	328	VAL	LEU	conflict	UNP Q9WTK5
F	328	VAL	LEU	conflict	UNP Q9WTK5

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



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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	29	Total	O	0	0
			29	29		
4	B	28	Total	O	0	0
			28	28		
4	C	28	Total	O	0	0
			28	28		

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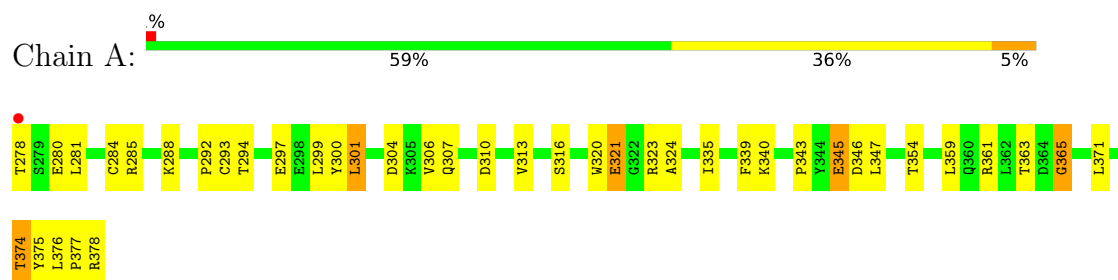
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	19	Total 19	O 19	0	0
4	E	21	Total 21	O 21	0	0
4	F	21	Total 21	O 21	0	0

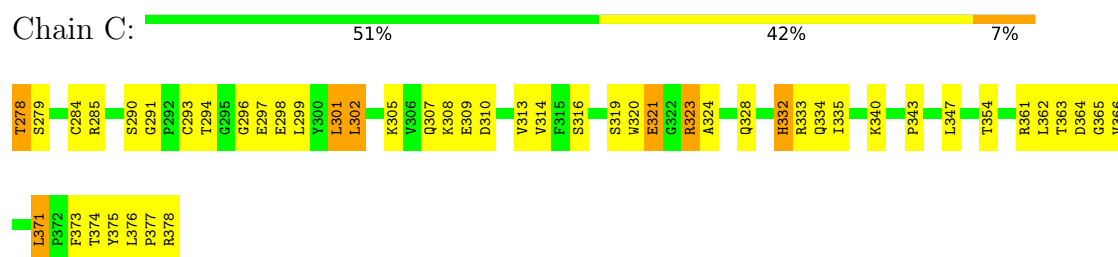
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

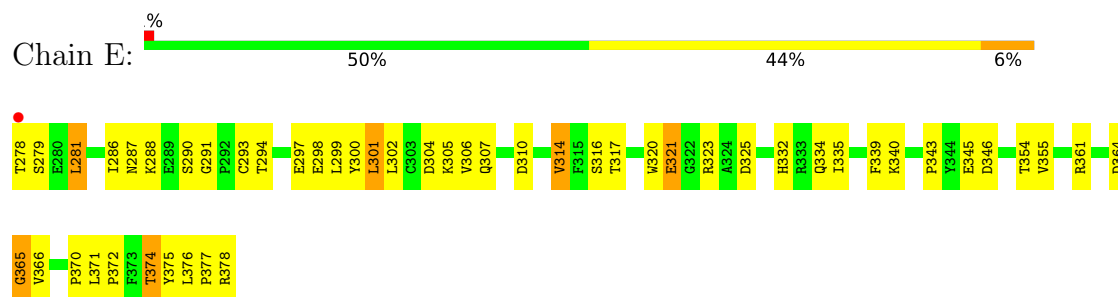
• Molecule 1: Transcription factor RelB



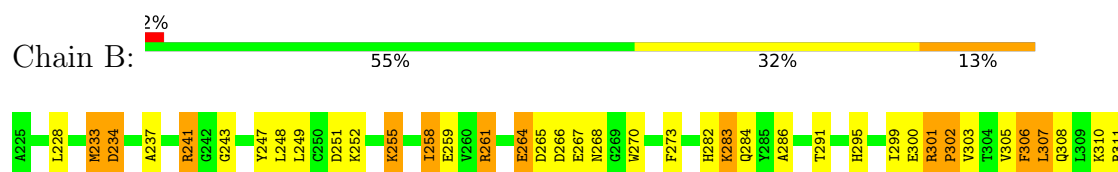
• Molecule 1: Transcription factor RelB

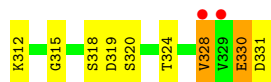


• Molecule 1: Transcription factor RelB



• Molecule 2: Nuclear factor NF-kappa-B p100 subunit





- Molecule 2: Nuclear factor NF-kappa-B p100 subunit



- Molecule 2: Nuclear factor NF-kappa-B p100 subunit



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	126.33Å 141.14Å 168.99Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.63 – 2.78 29.63 – 2.78	Depositor EDS
% Data completeness (in resolution range)	70.3 (29.63-2.78) 80.2 (29.63-2.78)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.27 (at 2.77Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.205 , 0.248 0.223 , 0.263	Depositor DCC
R_{free} test set	1676 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	44.8	Xtriage
Anisotropy	1.343	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 57.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	5191	wwPDB-VP
Average B, all atoms (Å ²)	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.10% 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	0.43	0/817	0.99	1/1111 (0.1%)
1	C	0.40	0/817	0.97	3/1111 (0.3%)
1	E	0.42	0/817	1.02	4/1111 (0.4%)
2	B	0.42	0/895	1.00	5/1206 (0.4%)
2	D	0.38	0/887	0.98	3/1195 (0.3%)
2	F	0.40	0/878	0.96	4/1183 (0.3%)
All	All	0.41	0/5111	0.99	20/6917 (0.3%)

There are no bond length outliers.

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	316	SER	N-CA-C	7.36	120.05	108.79
1	E	316	SER	N-CA-C	7.17	119.04	108.14
2	D	282	HIS	N-CA-C	6.90	119.09	109.15
1	C	316	SER	N-CA-C	6.90	119.35	108.79
1	E	332	HIS	N-CA-C	6.33	118.27	109.15
2	D	261	ARG	N-CA-C	6.21	118.54	108.41
2	B	315	GLY	N-CA-C	-5.84	107.04	115.27
1	C	314	VAL	N-CA-C	5.79	116.21	108.11
1	E	372	PRO	N-CA-C	5.72	119.44	110.80
2	B	233	MET	N-CA-C	5.60	117.35	107.61
2	B	258	ILE	N-CA-C	5.58	117.77	109.17
1	C	332	HIS	N-CA-C	5.58	117.19	109.15
2	F	315	GLY	N-CA-C	-5.47	107.56	115.27
2	D	309	LEU	N-CA-C	-5.32	102.61	110.48
2	F	233	MET	N-CA-C	5.31	116.99	107.80
2	F	258	ILE	N-CA-C	5.27	117.14	108.97
2	B	261	ARG	N-CA-C	5.24	117.51	109.07
2	F	261	ARG	N-CA-C	5.07	117.24	109.07

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Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	E	314	VAL	N-CA-C	5.02	115.14	108.11
2	B	282	HIS	N-CA-C	5.01	116.95	109.59

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	800	0	785	35	0
1	C	800	0	785	52	0
1	E	800	0	785	51	0
2	B	875	0	850	41	0
2	D	867	0	846	31	0
2	F	858	0	840	27	0
3	A	5	0	0	0	0
3	B	10	0	0	1	0
3	C	5	0	0	1	0
3	D	10	0	0	0	0
3	E	5	0	0	0	0
3	F	10	0	0	0	0
4	A	29	0	0	0	0
4	B	28	0	0	2	0
4	C	28	0	0	0	0
4	D	19	0	0	1	0
4	E	21	0	0	1	0
4	F	21	0	0	0	0
All	All	5191	0	4891	232	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 23.

All (232) 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:A:354:THR:HG22	1:A:374:THR:HB	1.44	0.99
2:B:301:ARG:HH11	2:B:301:ARG:HB3	1.26	0.98
1:C:378:ARG:HB3	1:C:378:ARG:NH1	1.82	0.93
1:C:378:ARG:HB3	1:C:378:ARG:HH11	1.33	0.92
2:D:234:ASP:HB2	2:D:247:TYR:H	1.39	0.88
1:E:323:ARG:HH21	1:E:323:ARG:HG3	1.46	0.80
1:A:354:THR:HG22	1:A:374:THR:CB	2.14	0.78
1:A:377:PRO:O	1:A:378:ARG:HB2	1.82	0.78
1:C:320:TRP:CG	1:C:321:GLU:H	2.05	0.75
2:B:234:ASP:HB2	2:B:247:TYR:HB2	1.69	0.74
2:F:228:LEU:HD21	2:F:311:ARG:NH1	2.02	0.74
2:F:234:ASP:HB2	2:F:247:TYR:HB2	1.69	0.73
2:B:233:MET:HE2	2:B:248:LEU:HD12	1.71	0.73
1:C:310:ASP:CG	1:C:363:THR:HG23	2.13	0.72
1:E:299:LEU:HB2	1:E:339:PHE:CE1	2.24	0.71
1:E:378:ARG:HG2	1:E:378:ARG:HH11	1.56	0.70
1:C:290:SER:HB2	1:C:376:LEU:HD21	1.71	0.70
1:E:377:PRO:O	1:E:378:ARG:HB3	1.90	0.70
1:C:320:TRP:CG	1:C:321:GLU:N	2.61	0.67
1:E:323:ARG:HG3	1:E:323:ARG:NH2	2.10	0.67
1:E:354:THR:HG22	1:E:374:THR:CG2	2.23	0.67
1:C:354:THR:HB	1:C:374:THR:HG22	1.77	0.66
1:C:307:GLN:HE21	1:C:307:GLN:HA	1.59	0.66
1:C:310:ASP:OD1	1:C:363:THR:HG23	1.96	0.66
1:C:307:GLN:HA	1:C:307:GLN:NE2	2.11	0.66
1:E:290:SER:HB2	1:E:376:LEU:HD11	1.78	0.66
1:E:354:THR:HG22	1:E:374:THR:HB	1.78	0.66
2:F:234:ASP:CB	2:F:247:TYR:H	2.08	0.65
1:E:297:GLU:O	1:E:340:LYS:HA	1.97	0.64
2:B:259:GLU:OE1	2:B:273:PHE:HE1	1.81	0.63
1:A:310:ASP:OD1	1:A:363:THR:HG23	1.99	0.63
1:A:320:TRP:CG	1:A:321:GLU:H	2.16	0.63
1:E:294:THR:O	1:E:343:PRO:HB3	1.98	0.63
1:A:320:TRP:CG	1:A:321:GLU:N	2.67	0.63
2:F:241:ARG:HG3	2:F:297:MET:HE1	1.80	0.63
2:B:259:GLU:OE2	2:B:312:LYS:HG2	1.99	0.63
1:A:301:LEU:HD12	1:A:301:LEU:C	2.24	0.62
1:C:301:LEU:HD12	1:C:301:LEU:O	1.99	0.62
2:D:234:ASP:HB3	2:D:235:LYS:HD2	1.81	0.62
1:C:364:ASP:CG	1:C:366:VAL:HG23	2.24	0.61
1:E:320:TRP:CG	1:E:321:GLU:H	2.18	0.61
1:E:320:TRP:CG	1:E:321:GLU:N	2.68	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:301:LEU:HD12	1:A:301:LEU:O	1.99	0.61
2:B:306:PHE:N	2:B:306:PHE:CD2	2.68	0.61
1:A:354:THR:HA	1:A:374:THR:HA	1.82	0.61
1:E:281:LEU:HD12	1:E:361:ARG:HH21	1.66	0.61
1:A:354:THR:CG2	1:A:374:THR:HB	2.27	0.60
1:C:354:THR:CB	1:C:374:THR:HG22	2.31	0.60
1:C:335:ILE:HD12	1:C:335:ILE:C	2.26	0.60
1:E:291:GLY:H	1:E:376:LEU:HD13	1.67	0.60
1:C:313:VAL:HB	1:C:324:ALA:HB3	1.84	0.59
1:E:361:ARG:O	1:E:365:GLY:HA2	2.02	0.59
2:B:299:ILE:HD12	2:B:303:VAL:HG23	1.84	0.59
1:C:297:GLU:O	1:C:340:LYS:HA	2.03	0.59
2:B:306:PHE:N	2:B:306:PHE:HD2	2.00	0.59
1:E:370:PRO:C	1:E:371:LEU:HD12	2.27	0.59
2:B:301:ARG:HB3	2:B:301:ARG:NH1	2.08	0.59
1:A:293:CYS:HA	1:A:375:TYR:CD2	2.38	0.58
2:B:234:ASP:CB	2:B:247:TYR:H	2.17	0.58
1:C:377:PRO:O	1:C:378:ARG:HB2	2.02	0.58
1:A:354:THR:HG22	1:A:374:THR:CG2	2.33	0.58
1:A:307:GLN:HE21	1:A:307:GLN:HA	1.69	0.58
2:F:233:MET:HE1	2:F:307:LEU:HD21	1.84	0.58
2:D:310:LYS:HE3	2:D:315:GLY:O	2.04	0.58
1:C:296:GLY:O	1:C:340:LYS:HD3	2.03	0.57
2:F:270:TRP:CD1	2:F:295:HIS:HB3	2.39	0.57
1:A:301:LEU:HD23	1:A:339:PHE:HE2	1.69	0.57
1:A:297:GLU:O	1:A:340:LYS:HA	2.04	0.57
1:A:292:PRO:HD2	1:A:297:GLU:OE2	2.05	0.56
1:A:307:GLN:HA	1:A:307:GLN:NE2	2.20	0.56
2:F:256:ASP:O	2:F:312:LYS:HE2	2.05	0.56
1:A:320:TRP:CD1	1:A:321:GLU:H	2.24	0.56
2:B:259:GLU:OE1	2:B:273:PHE:CE1	2.59	0.56
1:C:354:THR:HB	1:C:374:THR:CG2	2.36	0.55
1:C:294:THR:O	1:C:343:PRO:HB3	2.07	0.55
2:D:240:VAL:HG23	2:D:294:TYR:HB3	1.89	0.55
1:C:298:GLU:O	1:C:299:LEU:HD23	2.07	0.55
1:E:354:THR:HG22	1:E:374:THR:CB	2.36	0.55
1:A:300:TYR:CE2	2:B:234:ASP:HA	2.42	0.55
1:C:309:GLU:HA	1:C:328:GLN:NE2	2.20	0.55
1:C:320:TRP:O	1:C:321:GLU:HB2	2.07	0.55
1:C:308:LYS:HD2	1:C:328:GLN:HB3	1.88	0.54
1:C:293:CYS:HA	1:C:375:TYR:CD2	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:261:ARG:O	2:F:307:LEU:HA	2.07	0.54
1:E:307:GLN:HA	1:E:307:GLN:HE21	1.72	0.54
1:E:302:LEU:HD13	2:F:247:TYR:HE2	1.73	0.54
2:F:240:VAL:HG11	2:F:297:MET:HA	1.90	0.54
1:E:317:THR:CG2	1:E:355:VAL:HG12	2.38	0.54
1:E:370:PRO:O	1:E:371:LEU:HD12	2.08	0.53
1:A:335:ILE:C	1:A:335:ILE:HD12	2.33	0.53
1:C:321:GLU:HG2	1:C:323:ARG:HH21	1.73	0.53
2:B:258:ILE:HG13	2:B:259:GLU:N	2.24	0.53
2:B:305:VAL:C	2:B:306:PHE:HD2	2.17	0.53
2:D:281:VAL:HG22	2:D:287:ILE:HG12	1.89	0.53
1:C:291:GLY:H	1:C:376:LEU:CD2	2.21	0.53
1:E:354:THR:HA	1:E:374:THR:HA	1.90	0.53
1:E:293:CYS:HA	1:E:375:TYR:CD2	2.45	0.52
2:D:234:ASP:CB	2:D:247:TYR:H	2.17	0.52
1:E:317:THR:HG22	1:E:355:VAL:HG12	1.92	0.52
2:B:311:ARG:HD3	4:B:482:HOH:O	2.09	0.52
2:D:251:ASP:O	2:D:253:VAL:HG13	2.10	0.52
1:E:314:VAL:HG22	1:E:323:ARG:HG2	1.90	0.52
1:E:378:ARG:HG2	1:E:378:ARG:NH1	2.22	0.52
1:A:313:VAL:HB	1:A:324:ALA:HB3	1.92	0.52
2:D:307:LEU:HD23	2:D:323:PHE:HB2	1.92	0.52
2:F:240:VAL:HG12	2:F:297:MET:SD	2.51	0.51
1:E:299:LEU:HD12	1:E:339:PHE:HE1	1.76	0.51
2:D:235:LYS:HD3	2:D:246:VAL:HG22	1.91	0.51
1:E:307:GLN:HA	1:E:307:GLN:NE2	2.26	0.51
1:E:364:ASP:CG	1:E:366:VAL:HG23	2.36	0.51
1:E:278:THR:HG23	1:E:279:SER:H	1.76	0.51
2:F:248:LEU:C	2:F:248:LEU:HD23	2.35	0.51
1:C:301:LEU:HD12	1:C:301:LEU:C	2.35	0.51
2:B:261:ARG:O	2:B:307:LEU:HA	2.11	0.50
1:E:375:TYR:C	1:E:376:LEU:HD12	2.36	0.50
1:A:294:THR:O	1:A:343:PRO:HB3	2.12	0.50
2:B:234:ASP:HB3	2:B:247:TYR:H	1.77	0.50
1:C:332:HIS:CE1	1:C:333:ARG:HD3	2.47	0.50
1:C:320:TRP:CD1	1:C:321:GLU:H	2.28	0.50
1:E:300:TYR:CE1	2:F:234:ASP:HA	2.45	0.50
1:C:305:LYS:HA	1:C:334:GLN:O	2.12	0.50
2:D:234:ASP:HB2	2:D:247:TYR:N	2.18	0.50
1:E:301:LEU:C	1:E:301:LEU:HD23	2.38	0.49
2:B:243:GLY:N	2:B:291:THR:O	2.38	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:270:TRP:CD1	2:B:295:HIS:HB3	2.47	0.49
2:B:301:ARG:N	2:B:301:ARG:HD2	2.27	0.49
2:F:307:LEU:HD21	2:F:321:LYS:HB2	1.93	0.49
1:C:321:GLU:HG2	1:C:323:ARG:NH2	2.27	0.49
1:C:376:LEU:N	1:C:376:LEU:HD22	2.28	0.48
2:F:258:ILE:HG13	2:F:259:GLU:N	2.28	0.48
1:E:298:GLU:O	1:E:299:LEU:HD23	2.13	0.48
1:E:320:TRP:CD1	1:E:345:GLU:HB2	2.48	0.48
2:B:299:ILE:CD1	2:B:303:VAL:HG23	2.43	0.48
2:F:302:PRO:HG3	2:F:326:TYR:HD1	1.78	0.47
2:B:301:ARG:HH11	2:B:301:ARG:CB	2.12	0.47
1:A:284:CYS:O	1:A:285:ARG:HB3	2.14	0.47
1:C:361:ARG:O	1:C:365:GLY:HA2	2.15	0.47
1:E:304:ASP:O	1:E:306:VAL:HG13	2.15	0.47
1:A:281:LEU:HD22	1:A:359:LEU:HB2	1.96	0.47
2:B:248:LEU:C	2:B:248:LEU:HD23	2.40	0.47
2:D:228:LEU:CB	2:D:318:SER:HB3	2.45	0.47
1:E:335:ILE:HD12	1:E:335:ILE:C	2.40	0.47
2:B:264:GLU:HG2	2:B:270:TRP:HE3	1.80	0.47
2:B:308:GLN:HB3	2:B:320:SER:HB3	1.97	0.47
2:B:258:ILE:HD12	2:B:310:LYS:O	2.15	0.46
2:B:330:GLU:O	2:B:331:ASP:HB2	2.15	0.46
1:C:333:ARG:HD2	3:C:605:SO4:O4	2.15	0.46
1:A:301:LEU:HD23	1:A:339:PHE:CE2	2.49	0.46
1:C:291:GLY:H	1:C:376:LEU:HD23	1.80	0.46
2:D:261:ARG:O	2:D:307:LEU:HA	2.16	0.46
1:A:293:CYS:HA	1:A:375:TYR:HD2	1.79	0.46
1:C:307:GLN:HE21	1:C:307:GLN:CA	2.22	0.46
1:E:320:TRP:O	1:E:321:GLU:HB2	2.16	0.46
2:D:235:LYS:HD2	2:D:235:LYS:N	2.30	0.46
2:D:243:GLY:N	2:D:291:THR:O	2.48	0.46
2:D:306:PHE:HA	2:D:321:LYS:O	2.15	0.46
1:C:284:CYS:O	1:C:285:ARG:HB3	2.16	0.46
2:B:300:GLU:OE1	2:B:300:GLU:HA	2.16	0.46
1:C:302:LEU:CD2	2:D:247:TYR:CE2	2.99	0.46
1:A:307:GLN:HE21	1:A:307:GLN:CA	2.26	0.45
1:C:375:TYR:C	1:C:376:LEU:HD22	2.41	0.45
2:D:254:GLN:HB3	4:D:440:HOH:O	2.17	0.45
2:F:234:ASP:HB2	2:F:247:TYR:H	1.79	0.45
1:C:354:THR:HA	1:C:374:THR:HA	1.98	0.45
2:B:255:LYS:HD2	3:B:607:SO4:O1	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:373:PHE:CD1	1:C:373:PHE:C	2.95	0.45
1:E:339:PHE:C	1:E:339:PHE:CD1	2.95	0.45
1:A:304:ASP:O	1:A:306:VAL:HG13	2.16	0.44
1:C:294:THR:HA	1:C:347:LEU:HD22	1.99	0.44
2:D:258:ILE:HG13	2:D:259:GLU:N	2.31	0.44
1:E:320:TRP:CD1	1:E:321:GLU:H	2.34	0.44
2:F:313:ARG:HH21	2:F:313:ARG:HG2	1.82	0.44
1:C:332:HIS:CD2	2:D:249:LEU:HB3	2.52	0.44
1:A:288:LYS:HB2	1:A:299:LEU:HD22	1.98	0.44
2:D:318:SER:O	2:D:319:ASP:C	2.59	0.44
2:B:241:ARG:HB2	2:B:241:ARG:HH11	1.82	0.44
1:C:291:GLY:N	1:C:376:LEU:HD23	2.33	0.44
2:F:233:MET:O	2:F:234:ASP:C	2.61	0.44
2:B:264:GLU:OE2	2:B:295:HIS:HE1	2.00	0.44
1:E:286:ILE:HG22	1:E:288:LYS:O	2.18	0.44
2:D:253:VAL:HG22	2:D:284:GLN:O	2.18	0.44
1:E:301:LEU:HD23	1:E:301:LEU:O	2.18	0.44
2:F:252:LYS:HE3	2:F:284:GLN:NE2	2.33	0.44
1:E:361:ARG:HE	1:E:361:ARG:HB2	1.58	0.43
2:D:280:ASP:HB3	2:D:288:VAL:O	2.18	0.43
2:F:281:VAL:HG22	2:F:287:ILE:HG12	2.00	0.43
2:B:328:VAL:O	2:B:328:VAL:HG13	2.18	0.43
1:C:291:GLY:O	1:C:375:TYR:HA	2.18	0.43
1:A:345:GLU:HG2	1:A:346:ASP:N	2.28	0.43
2:B:302:PRO:HB2	4:B:507:HOH:O	2.19	0.43
1:C:278:THR:HG23	1:C:279:SER:H	1.83	0.43
2:B:249:LEU:HD23	2:B:286:ALA:HB2	2.01	0.43
1:C:335:ILE:C	1:C:335:ILE:CD1	2.92	0.42
2:F:240:VAL:HG13	2:F:294:TYR:HB3	2.01	0.42
1:A:320:TRP:O	1:A:321:GLU:HB2	2.19	0.42
1:E:346:ASP:OD1	1:E:346:ASP:C	2.62	0.42
2:B:237:ALA:HA	2:B:324:THR:O	2.20	0.42
2:D:261:ARG:HD2	2:D:273:PHE:HE1	1.85	0.42
2:B:266:ASP:OD1	2:B:268:ASN:HB3	2.20	0.42
1:C:371:LEU:HD12	1:C:371:LEU:HA	1.76	0.42
1:A:294:THR:HA	1:A:347:LEU:HD22	2.01	0.41
1:C:293:CYS:HA	1:C:375:TYR:HD2	1.85	0.41
1:E:323:ARG:NH2	1:E:323:ARG:CG	2.81	0.41
2:B:228:LEU:HD21	2:B:311:ARG:CZ	2.51	0.41
2:D:234:ASP:OD1	2:D:247:TYR:HB2	2.21	0.41
1:E:310:ASP:OD2	1:E:361:ARG:CG	2.67	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:323:ARG:HD3	4:E:449:HOH:O	2.20	0.41
2:B:295:HIS:CD2	2:B:295:HIS:C	2.98	0.41
1:C:299:LEU:HD11	1:C:373:PHE:CE2	2.56	0.41
2:D:303:VAL:O	2:D:324:THR:HG23	2.21	0.41
1:E:302:LEU:HD12	1:E:302:LEU:N	2.36	0.41
1:A:361:ARG:O	1:A:365:GLY:HA2	2.20	0.41
2:F:243:GLY:N	2:F:291:THR:O	2.44	0.41
1:C:378:ARG:HH11	1:C:378:ARG:CB	2.19	0.41
1:E:286:ILE:HG22	1:E:288:LYS:H	1.84	0.41
2:F:234:ASP:HB3	2:F:247:TYR:H	1.81	0.41
2:F:307:LEU:CD2	2:F:321:LYS:HB2	2.51	0.41
1:A:378:ARG:NH1	1:A:378:ARG:HG2	2.36	0.41
2:D:235:LYS:HD2	2:D:235:LYS:H	1.85	0.41
2:D:257:ASP:OD2	2:D:311:ARG:HB2	2.21	0.41
2:F:241:ARG:HG3	2:F:297:MET:CE	2.47	0.41
2:B:318:SER:O	2:B:319:ASP:C	2.64	0.41
2:D:228:LEU:HB3	2:D:318:SER:HB3	2.03	0.41
2:D:279:THR:C	2:D:281:VAL:H	2.28	0.41
2:F:234:ASP:HB2	2:F:247:TYR:CB	2.44	0.41
2:B:283:LYS:O	2:B:284:GLN:HB2	2.22	0.40
1:E:287:ASN:CG	1:E:300:TYR:H	2.29	0.40
1:A:301:LEU:C	1:A:301:LEU:CD1	2.93	0.40
2:D:306:PHE:HB3	2:D:320:SER:HB2	2.02	0.40
2:D:291:THR:HG21	2:D:323:PHE:CZ	2.56	0.40
2:B:267:GLU:O	2:B:268:ASN:C	2.65	0.40
1:E:305:LYS:HA	1:E:334:GLN:O	2.21	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	99/101 (98%)	86 (87%)	11 (11%)	2 (2%)	6	18
1	C	99/101 (98%)	89 (90%)	9 (9%)	1 (1%)	12	35
1	E	99/101 (98%)	85 (86%)	12 (12%)	2 (2%)	6	18
2	B	105/107 (98%)	90 (86%)	7 (7%)	8 (8%)	1	1
2	D	104/107 (97%)	92 (88%)	8 (8%)	4 (4%)	2	7
2	F	103/107 (96%)	92 (89%)	7 (7%)	4 (4%)	2	7
All	All	609/624 (98%)	534 (88%)	54 (9%)	21 (3%)	3	9

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	321	GLU
2	D	280	ASP
1	E	321	GLU
1	A	321	GLU
1	A	365	GLY
2	B	234	ASP
2	B	255	LYS
2	B	330	GLU
2	D	234	ASP
2	F	234	ASP
2	F	255	LYS
2	B	252	LYS
2	B	265	ASP
2	B	283	LYS
2	D	255	LYS
2	F	252	LYS
2	B	302	PRO
2	D	313	ARG
1	E	365	GLY
2	F	302	PRO
2	B	328	VAL

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	92/92 (100%)	84 (91%)	8 (9%)	9	27
1	C	92/92 (100%)	85 (92%)	7 (8%)	12	33
1	E	92/92 (100%)	88 (96%)	4 (4%)	26	57
2	B	96/96 (100%)	90 (94%)	6 (6%)	16	41
2	D	95/96 (99%)	89 (94%)	6 (6%)	16	41
2	F	94/96 (98%)	91 (97%)	3 (3%)	34	67
All	All	561/564 (100%)	527 (94%)	34 (6%)	17	43

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	278	THR
1	A	280	GLU
1	A	301	LEU
1	A	323	ARG
1	A	345	GLU
1	A	371	LEU
1	A	374	THR
1	A	376	LEU
2	B	241	ARG
2	B	251	ASP
2	B	264	GLU
2	B	301	ARG
2	B	306	PHE
2	B	307	LEU
1	C	278	THR
1	C	301	LEU
1	C	302	LEU
1	C	319	SER
1	C	323	ARG
1	C	362	LEU
1	C	371	LEU
2	D	234	ASP
2	D	235	LYS
2	D	245	GLU
2	D	268	ASN
2	D	305	VAL
2	D	313	ARG
1	E	281	LEU
1	E	301	LEU
1	E	325	ASP

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Mol	Chain	Res	Type
1	E	374	THR
2	F	251	ASP
2	F	279	THR
2	F	301	ARG

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

Mol	Chain	Res	Type
1	A	307	GLN
1	A	328	GLN
1	A	356	ASN
2	B	254	GLN
2	B	268	ASN
2	B	295	HIS
1	C	307	GLN
1	C	328	GLN
1	C	332	HIS
1	C	356	ASN
2	D	268	ASN
2	D	295	HIS
2	D	322	GLN
1	E	307	GLN
1	E	328	GLN
1	E	356	ASN
2	F	295	HIS
2	F	308	GLN
2	F	322	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 [i](#)

9 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	SO4	A	606	-	4,4,4	0.86	0	6,6,6	0.08	0
3	SO4	E	604	-	4,4,4	0.83	0	6,6,6	0.09	0
3	SO4	B	601	-	4,4,4	0.95	0	6,6,6	0.07	0
3	SO4	F	602	-	4,4,4	0.95	0	6,6,6	0.11	0
3	SO4	B	607	-	4,4,4	1.26	0	6,6,6	0.07	0
3	SO4	C	605	-	4,4,4	0.84	0	6,6,6	0.09	0
3	SO4	F	609	-	4,4,4	1.38	0	6,6,6	0.08	0
3	SO4	D	603	-	4,4,4	0.88	0	6,6,6	0.08	0
3	SO4	D	608	-	4,4,4	1.38	0	6,6,6	0.13	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.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	607	SO4	1	0
3	C	605	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 [i](#)

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	101/101 (100%)	-0.17	1 (0%) 79 74	37, 63, 101, 117	0
1	C	101/101 (100%)	-0.04	0 100 100	39, 67, 97, 114	0
1	E	101/101 (100%)	0.15	1 (0%) 79 74	46, 73, 104, 120	0
2	B	107/107 (100%)	0.10	2 (1%) 66 59	39, 69, 122, 140	0
2	D	106/107 (99%)	0.17	2 (1%) 66 59	43, 76, 129, 139	0
2	F	105/107 (98%)	0.25	3 (2%) 53 46	44, 74, 124, 139	0
All	All	621/624 (99%)	0.08	9 (1%) 73 67	37, 71, 119, 140	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	329	VAL	3.9
2	D	225	ALA	3.4
1	A	278	THR	3.4
2	B	328	VAL	3.4
1	E	278	THR	3.2
2	B	329	VAL	2.6
2	F	241	ARG	2.3
2	F	225	ALA	2.2
2	D	297	MET	2.1

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	SO4	D	608	5/5	0.80	0.15	24,29,37,90	5
3	SO4	B	607	5/5	0.83	0.20	25,27,35,75	5
3	SO4	F	609	5/5	0.88	0.14	23,30,34,92	5
3	SO4	D	603	5/5	0.91	0.10	41,43,45,60	5
3	SO4	A	606	5/5	0.91	0.12	41,41,48,56	5
3	SO4	C	605	5/5	0.91	0.09	42,49,55,59	5
3	SO4	F	602	5/5	0.92	0.10	30,37,41,49	5
3	SO4	E	604	5/5	0.94	0.09	40,40,46,47	5
3	SO4	B	601	5/5	0.95	0.09	31,39,41,49	5

6.5 Other polymers [i](#)

There are no such residues in this entry.