



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 10:37 AM UTC

PDB ID : 4TRQ / pdb_00004trq
Title : Crystal structure of Sac3/Thp1/Sem1
Authors : Hellerschmied, D.; Schneider, S.; Kohler, A.; Clausen, T.
Deposited on : 2014-06-17
Resolution : 3.10 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

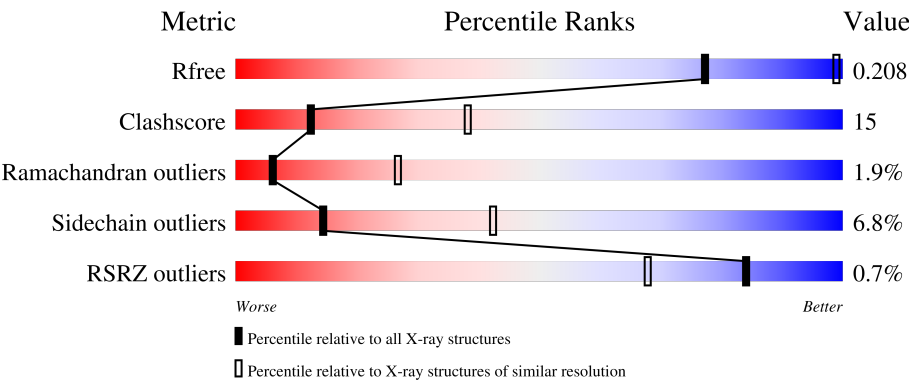
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)

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	299	% 64%30%5%•
1	D	299	61%30%7%•
2	B	286	72%24%•
2	E	286	% 67%29%•
3	C	60	53%17%12%18%

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Mol	Chain	Length	Quality of chain
3	F	60	5% 47% 30% 5% 18%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10521 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 Nuclear mRNA export protein SAC3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	299	Total	C	N	O	S	0	0	0
			2474	1582	426	453	13			
1	D	299	Total	C	N	O	S	0	0	0
			2474	1582	426	453	13			

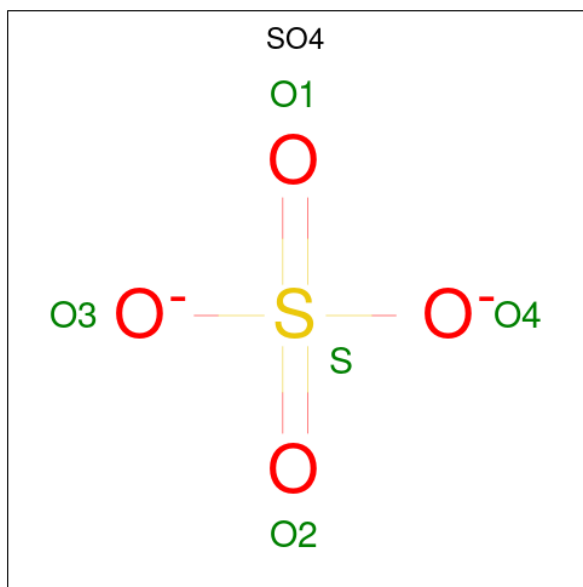
- Molecule 2 is a protein called Nuclear mRNA export protein THP1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	286	Total	C	N	O	S	0	0	0
			2359	1533	410	406	10			
2	E	286	Total	C	N	O	S	0	0	0
			2359	1533	410	406	10			

- Molecule 3 is a protein called 26S proteasome complex subunit SEM1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	49	Total	C	N	O	0	0	0
			425	260	65	100			
3	F	49	Total	C	N	O	0	0	0
			425	260	65	100			

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O₄S).

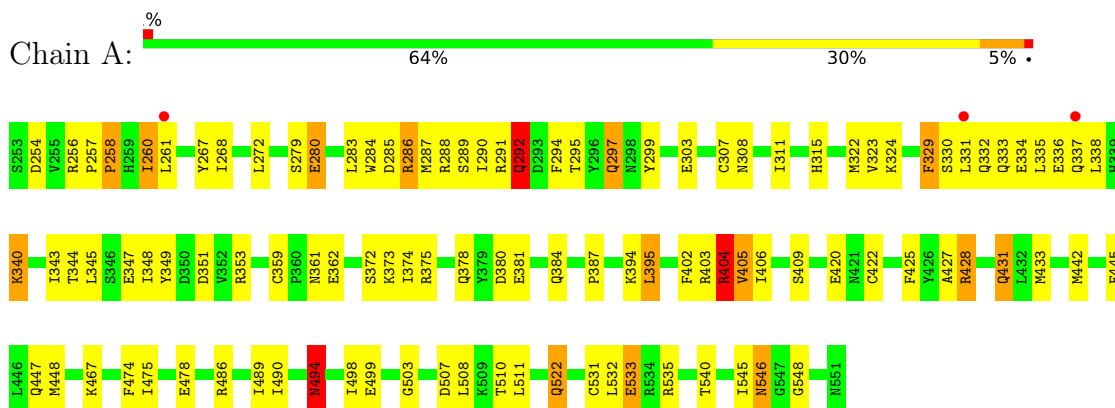


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		

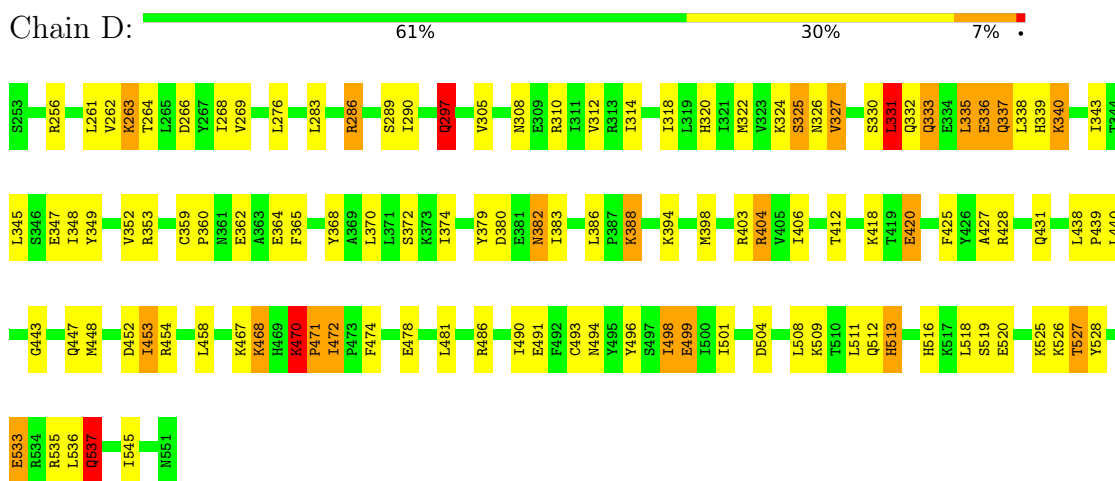
3 Residue-property plots

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.

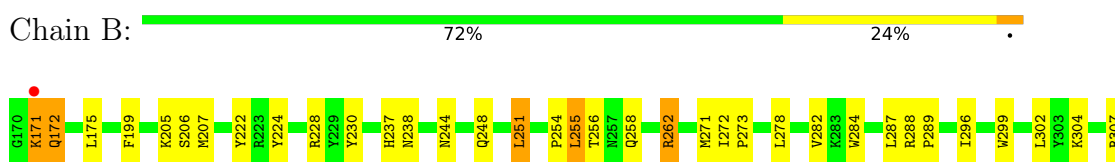
• Molecule 1: Nuclear mRNA export protein SAC3

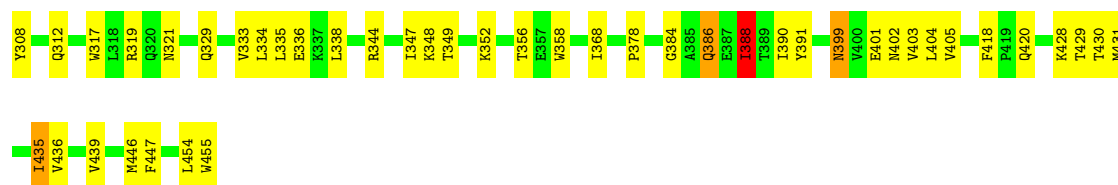


• Molecule 1: Nuclear mRNA export protein SAC3

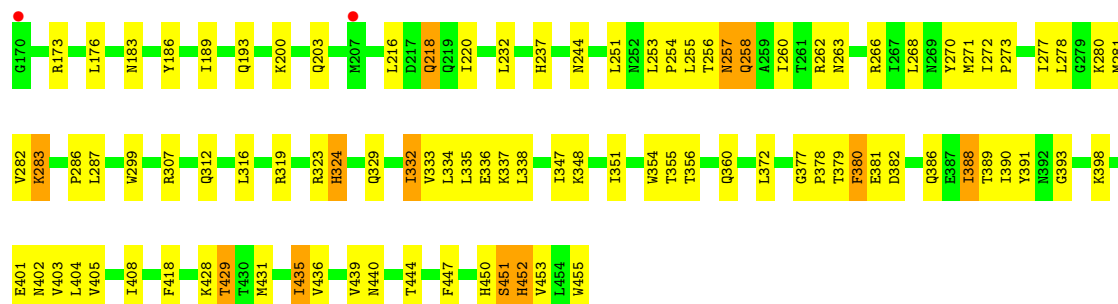


• Molecule 2: Nuclear mRNA export protein THP1

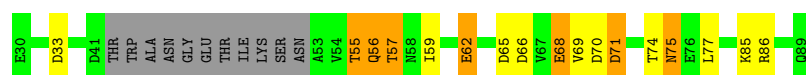




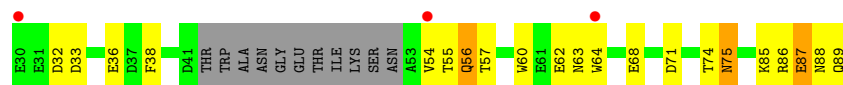
• Molecule 2: Nuclear mRNA export protein THP1



• Molecule 3: 26S proteasome complex subunit SEM1



• Molecule 3: 26S proteasome complex subunit SEM1



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	125.74Å 125.74Å 268.37Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.61 – 3.10 47.61 – 3.10	Depositor EDS
% Data completeness (in resolution range)	98.6 (47.61-3.10) 98.6 (47.61-3.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.84 (at 3.12Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, R_{free}	0.194 , 0.238 (Not available) , 0.208	Depositor DCC
R_{free} test set	1976 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	75.9	Xtriage
Anisotropy	0.167	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 67.1	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	0.94	EDS
Total number of atoms	10521	wwPDB-VP
Average B, all atoms (Å ²)	76.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.67% 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	0.47	0/2528	1.00	13/3415 (0.4%)
1	D	0.46	0/2528	1.00	12/3415 (0.4%)
2	B	0.48	0/2416	0.91	7/3282 (0.2%)
2	E	0.46	0/2416	0.97	6/3282 (0.2%)
3	C	0.52	0/432	1.07	1/584 (0.2%)
3	F	0.43	0/432	0.96	0/584
All	All	0.47	0/10752	0.98	39/14562 (0.3%)

There are no bond length outliers.

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	470	LYS	CA-C-N	9.81	132.10	119.84
1	D	470	LYS	C-N-CA	9.81	132.10	119.84
1	D	297	GLN	N-CA-C	7.68	121.75	112.38
1	A	333	GLN	N-CA-C	-7.60	104.11	113.15
3	C	33	ASP	N-CA-C	-7.37	102.67	114.09
1	A	292	GLN	N-CA-C	6.92	118.51	110.97
1	A	331	LEU	N-CA-C	-6.78	105.79	112.97
1	A	297	GLN	N-CA-C	-6.75	104.67	113.17
1	D	472	ILE	CA-C-N	6.65	126.69	119.90
1	D	472	ILE	C-N-CA	6.65	126.69	119.90
2	E	451	SER	CA-C-N	-6.42	112.29	122.95
2	E	451	SER	C-N-CA	-6.42	112.29	122.95
1	D	537	GLN	N-CA-C	6.33	118.99	111.71
2	E	324	HIS	N-CA-C	-6.29	105.25	113.17
1	A	545	ILE	CA-C-N	-6.12	113.40	122.83
1	A	545	ILE	C-N-CA	-6.12	113.40	122.83
1	A	404	ARG	CG-CD-NE	5.92	125.03	112.00
1	D	335	LEU	N-CA-C	5.87	117.75	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	418	PHE	CA-C-N	5.64	125.75	119.32
2	E	418	PHE	C-N-CA	5.64	125.75	119.32
1	A	338	LEU	N-CA-C	-5.54	105.32	111.36
1	A	404	ARG	CB-CG-CD	-5.51	98.63	111.30
1	A	494	ASN	N-CA-C	-5.46	105.74	112.90
1	A	359	CYS	CA-C-N	5.32	125.40	119.87
1	A	359	CYS	C-N-CA	5.32	125.40	119.87
2	B	251	LEU	CA-C-N	-5.27	114.38	122.60
2	B	251	LEU	C-N-CA	-5.27	114.38	122.60
1	A	280	GLU	N-CA-C	-5.19	106.45	112.89
1	D	333	GLN	N-CA-C	5.17	118.37	111.75
1	D	359	CYS	CA-C-N	5.16	126.29	119.84
1	D	359	CYS	C-N-CA	5.16	126.29	119.84
2	B	272	ILE	CA-C-N	-5.13	113.75	119.19
2	B	272	ILE	C-N-CA	-5.13	113.75	119.19
2	B	388	ILE	CB-CA-C	-5.08	103.62	111.08
2	B	418	PHE	CA-C-N	5.07	124.68	119.05
2	B	418	PHE	C-N-CA	5.07	124.68	119.05
1	D	512	GLN	CA-C-N	-5.03	115.39	122.94
1	D	512	GLN	C-N-CA	-5.03	115.39	122.94
2	E	439	VAL	N-CA-C	5.02	116.35	110.62

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	2474	0	2473	95	0
1	D	2474	0	2473	96	0
2	B	2359	0	2428	56	0
2	E	2359	0	2428	78	0
3	C	425	0	355	12	1
3	F	425	0	355	20	1
4	A	5	0	0	0	0
All	All	10521	0	10512	323	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 15.

All (323) 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:D:513:HIS:HD2	1:D:518:LEU:HD22	1.26	1.00
1:A:490:ILE:O	1:A:494:ASN:ND2	2.02	0.92
1:D:388:LYS:HD3	2:E:323:ARG:HD2	1.55	0.87
1:D:513:HIS:CD2	1:D:518:LEU:HD22	2.12	0.84
1:A:322:MET:HE2	1:A:329:PHE:HB3	1.61	0.83
2:E:281:MET:SD	3:F:64:TRP:HZ2	2.06	0.79
1:A:427:ALA:HB1	2:B:399:ASN:HD22	1.46	0.79
1:A:494:ASN:H	1:A:494:ASN:HD22	1.28	0.78
2:E:283:LYS:NZ	3:F:62:GLU:OE1	2.17	0.77
1:A:494:ASN:HD22	1:A:494:ASN:N	1.82	0.77
3:F:32:ASP:OD1	3:F:33:ASP:N	2.18	0.75
2:E:282:VAL:HG21	2:E:287:LEU:HD11	1.71	0.72
1:D:467:LYS:HD2	1:D:468:LYS:N	2.03	0.72
2:E:266:ARG:NH1	3:F:32:ASP:O	2.21	0.72
2:E:257:ASN:HB3	2:E:260:ILE:HD13	1.71	0.72
2:B:429:THR:HG22	2:B:431:MET:H	1.54	0.72
1:A:467:LYS:H	1:A:467:LYS:HD2	1.56	0.71
1:A:546:ASN:N	1:A:546:ASN:HD22	1.89	0.71
2:B:399:ASN:N	2:B:399:ASN:OD1	2.21	0.71
1:D:448:MET:O	1:D:526:LYS:NZ	2.22	0.71
2:E:244:ASN:HA	2:E:271:MET:HE3	1.72	0.71
2:E:257:ASN:OD1	2:E:258:GLN:N	2.23	0.71
1:D:336:GLU:HA	1:D:339:HIS:CD2	2.28	0.69
1:A:522:GLN:HA	1:A:522:GLN:OE1	1.91	0.68
1:D:276:LEU:HD13	1:D:283:LEU:HD12	1.77	0.67
1:A:373:LYS:O	1:A:375:ARG:N	2.27	0.67
1:A:288:ARG:HB2	1:A:337:GLN:HE22	1.61	0.66
2:B:175:LEU:HD11	2:B:207:MET:HE1	1.77	0.66
1:A:427:ALA:CB	2:B:399:ASN:HD22	2.08	0.66
1:A:349:TYR:CG	1:A:362:GLU:HG3	2.30	0.66
1:D:320:HIS:NE2	1:D:533:GLU:OE1	2.29	0.66
1:A:404:ARG:HE	2:B:336:GLU:HB2	1.62	0.65
1:A:291:ARG:HG3	1:A:308:ASN:OD1	1.97	0.64
3:F:75:ASN:H	3:F:75:ASN:HD22	1.46	0.64
1:A:478:GLU:HG3	1:A:489:ILE:HD11	1.77	0.64
1:A:499:GLU:H	1:A:510:THR:HG21	1.61	0.64
2:E:355:THR:HA	2:E:360:GLN:H	1.63	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:380:PHE:CE1	2:E:388:ILE:HG13	2.32	0.64
1:A:285:ASP:HB2	1:A:286:ARG:NH1	2.13	0.63
1:D:335:LEU:O	1:D:338:LEU:HB3	1.99	0.63
2:B:244:ASN:HA	2:B:271:MET:HE3	1.80	0.62
1:D:330:SER:CB	1:D:333:GLN:HB2	2.29	0.62
1:A:256:ARG:HD2	1:A:260:ILE:HD11	1.82	0.62
1:A:284:TRP:CZ2	1:A:337:GLN:HG3	2.34	0.62
1:D:406:ILE:HG12	1:D:453:ILE:HD11	1.82	0.62
1:D:425:PHE:HA	2:E:402:ASN:HD21	1.65	0.61
2:B:172:GLN:OE1	2:B:172:GLN:N	2.33	0.61
1:D:533:GLU:OE2	1:D:537:GLN:NE2	2.32	0.61
3:F:75:ASN:HD22	3:F:75:ASN:N	1.97	0.61
1:D:527:THR:OG1	1:D:528:TYR:N	2.33	0.61
2:E:281:MET:SD	3:F:64:TRP:CZ2	2.91	0.61
3:C:65:ASP:O	3:C:66:ASP:HB2	2.00	0.61
1:A:486:ARG:NH2	1:A:503:GLY:O	2.33	0.61
1:D:314:ILE:HG12	1:D:545:ILE:HG12	1.83	0.61
1:D:458:LEU:HD21	1:D:481:LEU:HD11	1.81	0.61
1:D:339:HIS:CE1	1:D:372:SER:HB2	2.36	0.61
3:F:71:ASP:O	3:F:75:ASN:ND2	2.34	0.60
3:C:56:GLN:HG3	3:C:57:THR:H	1.66	0.60
1:D:326:ASN:HD21	1:D:525:LYS:HZ2	1.49	0.60
2:B:334:LEU:O	2:B:338:LEU:HB2	2.01	0.60
1:A:395:LEU:HD12	1:A:442:MET:HE1	1.83	0.59
2:E:176:LEU:HB3	2:E:218:GLN:HE21	1.67	0.59
1:D:398:MET:HE3	1:D:438:LEU:HA	1.84	0.59
1:A:535:ARG:HH11	1:A:535:ARG:HG2	1.67	0.59
1:D:467:LYS:NZ	1:D:509:LYS:HE2	2.16	0.59
1:D:261:LEU:HD22	1:D:290:ILE:HG23	1.83	0.59
1:D:490:ILE:HG22	1:D:494:ASN:HD21	1.68	0.58
1:A:268:ILE:HA	1:A:272:LEU:HD13	1.85	0.58
1:D:330:SER:HB3	1:D:333:GLN:HB2	1.85	0.58
1:D:326:ASN:HD21	1:D:525:LYS:NZ	2.00	0.58
2:B:282:VAL:HG21	2:B:287:LEU:HD11	1.85	0.58
1:D:493:CYS:HB3	1:D:498:ILE:HB	1.86	0.58
2:E:401:GLU:O	2:E:405:VAL:HG23	2.03	0.58
2:B:258:GLN:O	2:B:262:ARG:HB2	2.04	0.57
1:D:256:ARG:NH2	1:D:289:SER:OG	2.36	0.57
2:E:266:ARG:HH21	3:F:36:GLU:HG3	1.69	0.57
2:E:312:GLN:HE21	2:E:377:GLY:HA3	1.69	0.57
2:E:351:ILE:HG21	2:E:435:ILE:HD13	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:283:LEU:HD12	1:A:283:LEU:H	1.69	0.57
1:D:498:ILE:O	1:D:499:GLU:HB2	2.02	0.57
1:D:340:LYS:HA	1:D:343:ILE:HG12	1.86	0.57
1:D:331:LEU:H	1:D:331:LEU:HD12	1.70	0.57
2:E:253:LEU:HD12	2:E:254:PRO:HD2	1.86	0.57
1:D:472:ILE:HD13	1:D:508:LEU:HG	1.87	0.57
1:D:324:LYS:HD3	1:D:533:GLU:CD	2.30	0.56
2:B:429:THR:HG22	2:B:431:MET:N	2.20	0.56
1:A:344:THR:O	1:A:348:ILE:HG12	2.06	0.56
2:E:273:PRO:HG3	2:E:299:TRP:CH2	2.41	0.56
1:D:353:ARG:NH2	1:D:362:GLU:OE1	2.38	0.56
1:D:471:PRO:HG3	1:D:501:ILE:HD12	1.88	0.56
2:E:379:THR:HG22	2:E:382:ASP:CG	2.31	0.56
1:A:330:SER:C	1:A:332:GLN:H	2.12	0.56
1:D:318:ILE:O	1:D:322:MET:HG2	2.05	0.56
2:E:335:LEU:HD21	2:E:390:ILE:HB	1.88	0.56
2:E:452:HIS:ND1	2:E:452:HIS:N	2.53	0.55
1:A:494:ASN:ND2	1:A:494:ASN:N	2.53	0.55
1:D:404:ARG:NH2	2:E:332:ILE:HD13	2.22	0.55
1:A:256:ARG:HB3	1:A:260:ILE:HD11	1.87	0.55
1:A:409:SER:N	1:A:422:CYS:HB2	2.22	0.55
1:A:336:GLU:N	1:A:336:GLU:OE1	2.37	0.54
1:A:427:ALA:HB3	2:B:402:ASN:HD22	1.73	0.54
1:D:339:HIS:HE1	1:D:372:SER:HB2	1.71	0.54
1:D:325:SER:HB2	1:D:327:VAL:HG12	1.90	0.54
1:D:420:GLU:O	2:E:337:LYS:HD2	2.06	0.54
2:E:183:ASN:HA	2:E:186:TYR:HD2	1.72	0.54
1:A:380:ASP:O	1:A:384:GLN:HG3	2.08	0.54
1:D:467:LYS:HD2	1:D:467:LYS:C	2.32	0.54
1:A:433:MET:HE2	1:A:433:MET:HA	1.90	0.54
1:D:533:GLU:O	1:D:536:LEU:HB3	2.07	0.54
1:D:308:ASN:O	1:D:312:VAL:HG23	2.08	0.53
1:D:348:ILE:O	1:D:352:VAL:HG23	2.08	0.53
1:A:261:LEU:HD22	1:A:290:ILE:HG12	1.90	0.53
1:A:332:GLN:C	1:A:334:GLU:H	2.16	0.53
2:B:386:GLN:HE21	2:B:386:GLN:N	2.07	0.53
2:E:272:ILE:HB	2:E:273:PRO:HD3	1.91	0.53
2:E:307:ARG:HE	3:F:64:TRP:CG	2.27	0.53
2:E:389:THR:HG23	2:E:391:TYR:H	1.72	0.53
1:D:269:VAL:HG11	1:D:310:ARG:NH2	2.24	0.53
2:B:237:HIS:HA	2:B:278:LEU:HD11	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:307:CYS:O	1:A:311:ILE:HG13	2.08	0.52
1:D:486:ARG:O	1:D:490:ILE:HG13	2.10	0.52
2:E:251:LEU:HD13	3:F:57:THR:HG21	1.91	0.52
1:D:314:ILE:O	1:D:318:ILE:HG13	2.09	0.52
1:D:326:ASN:ND2	1:D:525:LYS:NZ	2.58	0.51
3:C:62:GLU:CD	3:C:62:GLU:H	2.17	0.51
1:D:504:ASP:OD1	1:D:504:ASP:N	2.42	0.51
1:A:288:ARG:HG2	1:A:292:GLN:HE22	1.75	0.51
1:A:499:GLU:HG2	1:A:510:THR:HG21	1.91	0.51
2:B:388:ILE:HD13	2:B:388:ILE:H	1.75	0.51
1:D:491:GLU:HA	1:D:494:ASN:HD22	1.75	0.51
2:B:230:TYR:OH	2:B:455:TRP:O	2.20	0.51
1:D:452:ASP:HB3	1:D:516:HIS:CD2	2.46	0.51
1:A:315:HIS:ND1	1:A:334:GLU:OE2	2.38	0.51
3:C:56:GLN:HG3	3:C:57:THR:N	2.25	0.51
2:E:255:LEU:HD23	2:E:256:THR:H	1.75	0.51
2:E:270:TYR:O	2:E:273:PRO:HD2	2.11	0.51
1:A:261:LEU:HD22	1:A:290:ILE:HG23	1.93	0.51
1:D:496:TYR:HD1	1:D:518:LEU:HD21	1.75	0.51
1:A:256:ARG:CZ	1:A:261:LEU:HD21	2.41	0.51
3:F:85:LYS:O	3:F:89:GLN:HG3	2.11	0.51
1:A:286:ARG:HG2	1:A:286:ARG:HH11	1.76	0.50
2:E:263:ASN:HA	2:E:266:ARG:HD2	1.94	0.50
1:A:499:GLU:N	1:A:510:THR:HG21	2.26	0.50
1:D:438:LEU:HD12	1:D:439:PRO:HD2	1.93	0.50
2:B:224:TYR:CZ	2:B:228:ARG:HD2	2.47	0.50
1:D:335:LEU:HD21	1:D:448:MET:HE2	1.92	0.50
1:A:280:GLU:HA	1:A:283:LEU:HD13	1.93	0.50
1:A:288:ARG:HG2	1:A:292:GLN:NE2	2.28	0.49
1:A:380:ASP:CG	1:A:403:ARG:HH21	2.19	0.49
2:B:335:LEU:HD21	2:B:390:ILE:HB	1.93	0.49
2:E:200:LYS:HD2	2:E:203:GLN:HE22	1.77	0.49
3:F:87:GLU:O	3:F:89:GLN:N	2.44	0.49
1:A:427:ALA:CB	2:B:402:ASN:HD22	2.25	0.49
1:A:475:ILE:HD12	1:A:475:ILE:H	1.77	0.49
1:A:288:ARG:CB	1:A:337:GLN:HE22	2.24	0.49
1:A:427:ALA:H	2:B:402:ASN:ND2	2.11	0.49
1:D:404:ARG:HD2	2:E:336:GLU:HB2	1.94	0.49
1:A:405:VAL:HG22	1:A:425:PHE:HB2	1.93	0.49
1:D:332:GLN:NE2	1:D:333:GLN:HA	2.28	0.49
1:D:337:GLN:HA	1:D:340:LYS:HG3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:496:TYR:CD1	1:D:518:LEU:HD21	2.47	0.49
2:E:271:MET:HE2	3:F:60:TRP:HZ2	1.77	0.49
1:D:380:ASP:OD1	1:D:404:ARG:NH2	2.39	0.49
1:D:403:ARG:HB2	1:D:404:ARG:NH1	2.28	0.49
1:D:467:LYS:HZ3	1:D:509:LYS:HE2	1.76	0.49
2:B:348:LYS:HB2	2:B:436:VAL:HG11	1.94	0.49
2:B:244:ASN:HA	2:B:271:MET:CE	2.41	0.49
2:E:333:VAL:O	2:E:337:LYS:HG2	2.13	0.49
1:A:409:SER:H	1:A:422:CYS:HB2	1.78	0.48
1:D:404:ARG:HH21	2:E:332:ILE:CG2	2.25	0.48
2:E:380:PHE:CD1	2:E:380:PHE:C	2.90	0.48
1:D:345:LEU:HD22	1:D:349:TYR:CZ	2.48	0.48
1:D:474:PHE:O	1:D:478:GLU:HG3	2.12	0.48
2:B:344:ARG:HG2	2:B:344:ARG:HH11	1.78	0.48
2:E:351:ILE:HD13	2:E:435:ILE:HD11	1.94	0.48
1:D:337:GLN:HA	1:D:340:LYS:CG	2.44	0.48
2:E:336:GLU:OE1	2:E:337:LYS:HE3	2.13	0.48
1:D:427:ALA:O	1:D:431:GLN:HG3	2.13	0.48
1:D:498:ILE:HG12	1:D:511:LEU:HD13	1.96	0.48
1:A:343:ILE:O	1:A:347:GLU:HG3	2.14	0.48
1:D:382:ASN:N	1:D:382:ASN:HD22	2.12	0.48
1:A:351:ASP:N	1:A:351:ASP:OD1	2.46	0.47
2:B:388:ILE:HD13	2:B:388:ILE:N	2.28	0.47
2:E:277:ILE:HD11	2:E:334:LEU:HD23	1.96	0.47
2:E:312:GLN:HG2	2:E:316:LEU:HD13	1.96	0.47
3:C:55:THR:OG1	3:C:56:GLN:N	2.43	0.47
3:C:71:ASP:HA	3:C:75:ASN:ND2	2.29	0.47
1:A:507:ASP:O	1:A:510:THR:HG22	2.14	0.47
1:A:402:PHE:O	1:A:406:ILE:HG13	2.15	0.47
2:E:200:LYS:HD2	2:E:203:GLN:NE2	2.29	0.47
2:E:354:TRP:HD1	2:E:355:THR:HG22	1.79	0.47
1:A:373:LYS:HA	1:A:373:LYS:HE2	1.96	0.47
2:B:401:GLU:O	2:B:405:VAL:HG23	2.14	0.47
1:D:412:THR:HG22	1:D:418:LYS:HE2	1.96	0.47
1:A:332:GLN:HB3	1:A:335:LEU:HG	1.97	0.47
1:A:353:ARG:NH1	1:A:387:PRO:HG2	2.30	0.47
2:B:349:THR:HG21	3:C:77:LEU:HD23	1.97	0.47
1:D:428:ARG:HD3	2:E:393:GLY:O	2.15	0.47
2:E:268:LEU:O	2:E:272:ILE:HG12	2.15	0.47
1:A:372:SER:HA	1:A:445:PHE:CZ	2.50	0.47
2:E:429:THR:HG23	2:E:431:MET:H	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:370:LEU:HD23	1:D:379:TYR:HB3	1.96	0.46
1:A:353:ARG:CZ	1:A:387:PRO:HG2	2.46	0.46
1:D:343:ILE:O	1:D:347:GLU:HG2	2.16	0.46
2:E:200:LYS:HE3	2:E:200:LYS:HB3	1.78	0.46
1:A:256:ARG:NH2	1:A:289:SER:OG	2.49	0.46
1:A:257:PRO:HD2	1:A:260:ILE:HG12	1.97	0.46
1:A:258:PRO:HA	1:A:294:PHE:CE1	2.50	0.46
2:E:280:LYS:HG3	2:E:440:ASN:HD22	1.81	0.46
1:A:323:VAL:HG21	1:A:448:MET:HE1	1.98	0.46
1:D:364:GLU:HG2	1:D:368:TYR:CE2	2.51	0.46
1:D:263:LYS:HA	1:D:266:ASP:HB2	1.98	0.46
1:A:361:ASN:HD21	1:A:548:GLY:HA3	1.80	0.46
2:E:307:ARG:HG2	2:E:307:ARG:HH11	1.81	0.46
3:F:56:GLN:HB3	3:F:57:THR:H	1.50	0.46
2:B:254:PRO:O	2:B:256:THR:N	2.43	0.45
2:B:352:LYS:O	2:B:356:THR:OG1	2.28	0.45
3:C:57:THR:O	3:C:59:ILE:HG23	2.16	0.45
2:B:288:ARG:N	2:B:289:PRO:HD2	2.32	0.45
2:B:312:GLN:OE1	2:B:378:PRO:HD2	2.16	0.45
1:D:326:ASN:ND2	1:D:525:LYS:HZ3	2.13	0.45
1:D:268:ILE:HG23	1:D:283:LEU:HD22	1.99	0.45
1:D:382:ASN:HD22	1:D:382:ASN:H	1.65	0.45
3:F:68:GLU:HG2	3:F:74:THR:HG21	1.98	0.45
1:A:287:MET:HB3	1:A:311:ILE:HD13	1.98	0.45
2:E:273:PRO:HB3	2:E:334:LEU:HD21	1.98	0.45
2:E:404:LEU:O	2:E:408:ILE:HG13	2.17	0.45
1:D:383:ILE:HD12	1:D:386:LEU:HD12	1.99	0.45
2:E:312:GLN:NE2	2:E:377:GLY:HA3	2.30	0.45
2:E:355:THR:HG22	2:E:360:GLN:O	2.17	0.44
2:B:199:PHE:HB3	2:B:455:TRP:HA	1.99	0.44
2:B:273:PRO:HB3	2:B:299:TRP:CH2	2.51	0.44
1:D:264:THR:O	1:D:268:ILE:HG13	2.17	0.44
1:D:297:GLN:HE21	1:D:297:GLN:HB2	1.67	0.44
2:E:271:MET:HE2	3:F:60:TRP:CZ2	2.53	0.44
1:D:262:VAL:HG12	1:D:266:ASP:OD2	2.18	0.44
1:D:398:MET:CE	1:D:438:LEU:HA	2.47	0.44
1:A:299:TYR:HE2	1:A:303:GLU:HB2	1.82	0.44
2:E:266:ARG:NH2	3:F:36:GLU:HG3	2.32	0.44
1:A:532:LEU:HA	1:A:535:ARG:HD3	1.99	0.44
2:B:302:LEU:HB2	2:B:317:TRP:CE2	2.52	0.44
1:D:535:ARG:HG2	1:D:535:ARG:HH11	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:330:SER:HB2	1:D:333:GLN:HB2	1.97	0.44
2:E:216:LEU:O	2:E:220:ILE:HG13	2.17	0.44
2:E:312:GLN:NE2	2:E:378:PRO:HD2	2.33	0.44
2:B:284:TRP:O	2:B:288:ARG:HG3	2.17	0.44
2:B:344:ARG:HG2	2:B:344:ARG:NH1	2.33	0.43
2:B:430:THR:HB	2:B:431:MET:HE2	2.00	0.43
2:E:280:LYS:HG3	2:E:440:ASN:ND2	2.33	0.43
1:D:513:HIS:CD2	1:D:518:LEU:CD2	2.94	0.43
2:B:251:LEU:HA	2:B:255:LEU:HD21	1.99	0.43
2:B:308:TYR:OH	3:C:68:GLU:O	2.20	0.43
1:A:329:PHE:N	1:A:329:PHE:CD1	2.86	0.43
1:A:428:ARG:HA	1:A:431:GLN:OE1	2.18	0.43
1:A:258:PRO:HA	1:A:294:PHE:CZ	2.54	0.43
1:A:261:LEU:HD23	1:A:261:LEU:HA	1.78	0.43
2:B:368:ILE:HD12	2:B:404:LEU:HD11	2.00	0.43
2:B:308:TYR:OH	3:C:69:VAL:HA	2.19	0.43
1:A:378:GLN:O	1:A:381:GLU:HB3	2.19	0.43
2:B:222:TYR:CE1	2:B:454:LEU:HB3	2.54	0.43
2:B:319:ARG:HA	2:B:391:TYR:CZ	2.53	0.43
1:D:420:GLU:HB3	2:E:447:PHE:CD2	2.53	0.43
2:B:384:GLY:C	2:B:386:GLN:NE2	2.76	0.43
1:A:288:ARG:HB2	1:A:337:GLN:NE2	2.31	0.42
2:E:232:LEU:CD2	2:E:329:GLN:HG2	2.49	0.42
1:A:288:ARG:O	1:A:292:GLN:HB2	2.19	0.42
2:E:356:THR:HG22	2:E:429:THR:O	2.20	0.42
1:A:291:ARG:O	1:A:295:THR:HG23	2.19	0.42
1:D:403:ARG:CB	1:D:404:ARG:NH1	2.83	0.42
2:E:372:LEU:HD11	2:E:403:VAL:HG11	2.01	0.42
1:D:470:LYS:HA	1:D:471:PRO:HD2	1.73	0.42
1:D:336:GLU:O	1:D:340:LYS:HG2	2.20	0.42
1:D:458:LEU:HD21	1:D:481:LEU:CD1	2.45	0.42
2:E:283:LYS:O	2:E:286:PRO:HD2	2.20	0.42
2:E:354:TRP:NE1	2:E:360:GLN:HB3	2.34	0.42
1:A:427:ALA:HB1	2:B:399:ASN:ND2	2.25	0.42
2:B:284:TRP:CD2	2:B:296:ILE:HG23	2.54	0.42
1:D:452:ASP:HB3	1:D:516:HIS:HD2	1.82	0.42
2:B:230:TYR:CD2	2:B:238:ASN:HB3	2.54	0.42
1:A:381:GLU:HG3	2:B:329:GLN:OE1	2.20	0.41
1:A:498:ILE:HD11	1:A:511:LEU:HD22	2.02	0.41
2:B:254:PRO:C	2:B:256:THR:H	2.27	0.41
2:E:354:TRP:O	2:E:360:GLN:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:420:GLU:HG3	2:B:447:PHE:CG	2.54	0.41
2:B:446:MET:HE3	2:B:447:PHE:HE2	1.85	0.41
1:D:404:ARG:HH21	2:E:332:ILE:HG21	1.85	0.41
1:A:404:ARG:NE	2:B:336:GLU:OE1	2.54	0.41
1:D:443:GLY:O	1:D:447:GLN:HG3	2.20	0.41
1:A:404:ARG:HH11	1:A:404:ARG:HD3	1.76	0.41
1:A:474:PHE:O	1:A:478:GLU:HB2	2.20	0.41
2:B:171:LYS:HD2	2:B:171:LYS:HA	1.47	0.41
1:D:454:ARG:HG2	1:D:481:LEU:HD22	2.01	0.41
2:E:203:GLN:HB3	2:E:455:TRP:CZ2	2.56	0.41
2:E:237:HIS:HA	2:E:278:LEU:HD11	2.02	0.41
1:A:285:ASP:HB2	1:A:286:ARG:HH12	1.86	0.41
2:E:380:PHE:HE1	2:E:386:GLN:O	2.03	0.41
2:E:450:HIS:CG	2:E:451:SER:N	2.89	0.41
1:A:324:LYS:HE2	1:A:533:GLU:HG3	2.03	0.41
1:A:395:LEU:HD13	1:A:395:LEU:HA	1.79	0.41
1:A:508:LEU:HD23	1:A:508:LEU:HA	1.91	0.41
2:E:268:LEU:HD13	2:E:287:LEU:HD13	2.02	0.41
3:F:62:GLU:HG2	3:F:63:ASN:N	2.35	0.41
1:A:329:PHE:O	1:A:330:SER:HB3	2.21	0.41
1:A:447:GLN:OE1	1:A:532:LEU:HD12	2.20	0.41
1:D:286:ARG:O	1:D:290:ILE:HG13	2.21	0.41
2:E:319:ARG:HA	2:E:391:TYR:CZ	2.56	0.41
2:E:348:LYS:HB2	2:E:436:VAL:HG11	2.03	0.41
2:E:453:VAL:HG13	2:E:455:TRP:CE2	2.56	0.41
2:B:304:LYS:HD3	3:C:70:ASP:HB2	2.01	0.41
2:B:435:ILE:H	2:B:435:ILE:HG12	1.73	0.41
1:A:336:GLU:O	1:A:340:LYS:N	2.43	0.40
1:D:472:ILE:N	1:D:472:ILE:HD12	2.36	0.40
1:A:267:TYR:CE2	1:A:272:LEU:HD11	2.57	0.40
1:A:324:LYS:HG3	1:A:533:GLU:OE1	2.21	0.40
1:A:428:ARG:HA	1:A:431:GLN:HB2	2.02	0.40
2:B:358:TRP:CE3	3:C:85:LYS:HD3	2.57	0.40
2:E:338:LEU:HA	2:E:338:LEU:HD23	1.86	0.40
2:E:440:ASN:O	2:E:444:THR:HG23	2.22	0.40
3:F:54:VAL:O	3:F:56:GLN:N	2.54	0.40
1:A:345:LEU:HD22	1:A:349:TYR:CZ	2.57	0.40
1:D:349:TYR:CG	1:D:362:GLU:HG3	2.57	0.40
1:D:365:PHE:HA	1:D:368:TYR:HD2	1.86	0.40
2:E:193:GLN:OE1	2:E:193:GLN:N	2.54	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:86:ARG:NH2	3:F:38:PHE:O[5_445]	2.18	0.02

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	297/299 (99%)	273 (92%)	19 (6%)	5 (2%)	7	30
1	D	297/299 (99%)	266 (90%)	23 (8%)	8 (3%)	4	20
2	B	284/286 (99%)	261 (92%)	22 (8%)	1 (0%)	30	61
2	E	284/286 (99%)	258 (91%)	24 (8%)	2 (1%)	18	49
3	C	45/60 (75%)	33 (73%)	8 (18%)	4 (9%)	0	3
3	F	45/60 (75%)	36 (80%)	5 (11%)	4 (9%)	0	3
All	All	1252/1290 (97%)	1127 (90%)	101 (8%)	24 (2%)	6	27

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	374	ILE
3	C	56	GLN
3	C	71	ASP
1	D	468	LYS
1	D	499	GLU
3	F	56	GLN
1	A	254	ASP
1	A	531	CYS
3	C	68	GLU
1	D	519	SER
2	B	255	LEU
1	D	331	LEU
2	E	380	PHE

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Mol	Chain	Res	Type
3	F	55	THR
3	F	87	GLU
3	F	88	ASN
1	A	258	PRO
1	A	279	SER
1	D	471	PRO
2	E	398	LYS
3	C	55	THR
1	D	360	PRO
1	D	498	ILE
1	D	305	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	278/278 (100%)	261 (94%)	17 (6%)	17	46
1	D	278/278 (100%)	255 (92%)	23 (8%)	10	35
2	B	265/265 (100%)	247 (93%)	18 (7%)	14	42
2	E	265/265 (100%)	249 (94%)	16 (6%)	17	47
3	C	47/56 (84%)	43 (92%)	4 (8%)	10	35
3	F	47/56 (84%)	45 (96%)	2 (4%)	26	57
All	All	1180/1198 (98%)	1100 (93%)	80 (7%)	14	42

All (80) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	260	ILE
1	A	286	ARG
1	A	292	GLN
1	A	297	GLN
1	A	329	PHE
1	A	340	LYS
1	A	394	LYS

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Mol	Chain	Res	Type
1	A	395	LEU
1	A	404	ARG
1	A	405	VAL
1	A	428	ARG
1	A	431	GLN
1	A	494	ASN
1	A	522	GLN
1	A	533	GLU
1	A	540	THR
1	A	546	ASN
2	B	171	LYS
2	B	172	GLN
2	B	205	LYS
2	B	206	SER
2	B	248	GLN
2	B	262	ARG
2	B	307	ARG
2	B	321	ASN
2	B	333	VAL
2	B	347	ILE
2	B	386	GLN
2	B	388	ILE
2	B	399	ASN
2	B	403	VAL
2	B	420	GLN
2	B	428	LYS
2	B	435	ILE
2	B	439	VAL
3	C	57	THR
3	C	62	GLU
3	C	74	THR
3	C	75	ASN
1	D	263	LYS
1	D	286	ARG
1	D	297	GLN
1	D	325	SER
1	D	327	VAL
1	D	331	LEU
1	D	336	GLU
1	D	337	GLN
1	D	340	LYS
1	D	374	ILE

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Mol	Chain	Res	Type
1	D	382	ASN
1	D	388	LYS
1	D	394	LYS
1	D	404	ARG
1	D	420	GLU
1	D	440	LEU
1	D	453	ILE
1	D	470	LYS
1	D	513	HIS
1	D	520	GLU
1	D	527	THR
1	D	533	GLU
1	D	537	GLN
2	E	173	ARG
2	E	189	ILE
2	E	218	GLN
2	E	257	ASN
2	E	258	GLN
2	E	262	ARG
2	E	283	LYS
2	E	324	HIS
2	E	332	ILE
2	E	347	ILE
2	E	381	GLU
2	E	388	ILE
2	E	428	LYS
2	E	429	THR
2	E	435	ILE
2	E	452	HIS
3	F	75	ASN
3	F	86	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	259	HIS
1	A	271	ASN
1	A	292	GLN
1	A	297	GLN
1	A	332	GLN
1	A	337	GLN
1	A	361	ASN

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Mol	Chain	Res	Type
1	A	384	GLN
1	A	392	GLN
1	A	494	ASN
1	A	546	ASN
1	A	551	ASN
2	B	215	GLN
2	B	218	GLN
2	B	244	ASN
2	B	248	GLN
2	B	252	ASN
2	B	386	GLN
2	B	402	ASN
2	B	440	ASN
3	C	75	ASN
1	D	271	ASN
1	D	326	ASN
1	D	332	GLN
1	D	339	HIS
1	D	378	GLN
1	D	382	ASN
1	D	384	GLN
1	D	434	GLN
1	D	487	GLN
1	D	494	ASN
2	E	172	GLN
2	E	203	GLN
2	E	215	GLN
2	E	218	GLN
2	E	238	ASN
2	E	312	GLN
2	E	329	GLN
2	E	402	ASN
2	E	416	ASN
2	E	433	GLN
2	E	440	ASN
3	F	75	ASN

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](#)

1 ligand is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	SO4	A	601	-	4,4,4	0.32	0	6,6,6	0.15	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [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	299/299 (100%)	-0.37	3 (1%) 79 61	34, 65, 115, 169	0
1	D	299/299 (100%)	-0.08	0 100 100	50, 94, 139, 165	0
2	B	286/286 (100%)	-0.69	1 (0%) 90 80	30, 50, 83, 154	0
2	E	286/286 (100%)	-0.30	2 (0%) 84 68	40, 71, 110, 152	0
3	C	49/60 (81%)	0.03	0 100 100	45, 81, 138, 158	0
3	F	49/60 (81%)	0.18	3 (6%) 27 15	56, 100, 157, 180	0
All	All	1268/1290 (98%)	-0.32	9 (0%) 84 68	30, 72, 127, 180	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	170	GLY	4.1
3	F	64	TRP	3.7
2	B	171	LYS	3.4
1	A	331	LEU	2.4
1	A	337	GLN	2.3
3	F	30	GLU	2.2
1	A	261	LEU	2.2
3	F	54	VAL	2.2
2	E	207	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
4	SO4	A	601	5/5	0.90	0.09	88,90,96,107	0

6.5 Other polymers [i](#)

There are no such residues in this entry.